Page 1 of 1

STIC-EIC1600/2900

263877

From: Baek, Bong-Sook
Sent: Thursday, June 19, 2008 11:51 AM
To: STIC-EIC1600/2900
Subject: Search request for Application 10599913

Examiner: Bong-Sook (Francesca) Baek

RECEIVED
JUN 19 2008

Please search structure of claim 1 (see structure and description of R-groups in the attached claims).
Elected species 1-hydroxy-6-(2-morpholine-4-ylethoxy)-1,3-diphenyl-1H-indene-2- carboxylic acid ethyl ester
Further preferable examples are shown in claim 4 (See attached the claim document)

Keywords: modulator of peroxisome proliferator activated receptor (PPAR), treatment for diabetes, obesity, atherosclerosis, hyperlipidemia, hyperinsulinism, hypertension, osteoporosis, liver cirrhosis, asthma and cancer

If possible, please send a result before the next Thursday (6/26/2008)

Please send email or call me at 571-272-5863 if you have any questions.

Thank you

Bong-Sook (Francesca) Baek
Examiner
Patent Training Academy
Carlyle Center Room 3003

19
9/2008

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http://www.cas.org/support/stngen/stndoc/properties.html

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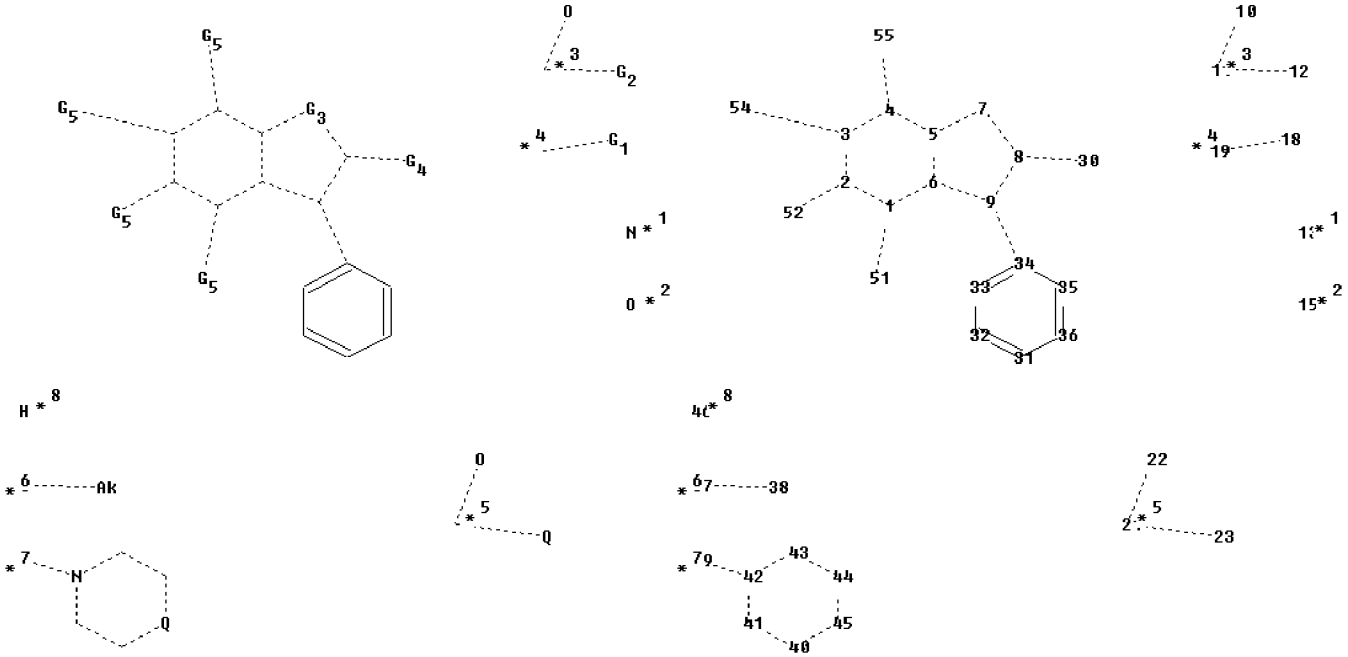

chain nodes :
10 12 15 18 21 22 23 30 37 38 39 46 51 52 54 55
ring nodes :
1 2 3 4 5 6 7 8 9 11 19 31 32 33 34 35 36 40 41 42 43 44 45

ring/chain nodes :
13
chain bonds :
1-51 2-52 3-54 4-55 8-30 9-34 10-11 11-12 18-19 21-22 21-23 37-38 39-42

ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9 31-32 31-36 32-33 33-34 34-35 35-36 40-41 40-45 41-42 42-43 43-44 44-45
exact/norm bonds :
1-2 1-6 1-51 2-3 2-52 3-4 3-54 4-5 4-55 5-6 5-7 6-9 7-8 8-9 8-30 9-34

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10-11  11-12  18-19  21-22  21-23  37-38  39-42  40-41  40-45  41-42  42-43  43-44
44-45
normalized bonds :
31-32  31-36  32-33  33-34  34-35  35-36


G1:[*1],[*2]

G2:Cb,Ak

G3:[*3],[*4]

G4:CN,[*5]

G5:[*6],[*7],[*8]

Connectivity :
21:3 E exact RC ring/chain  22:1 E exact RC ring/chain
Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  7:Atom  8:Atom  9:Atom  10:CLASS
11:Atom  12:CLASS  13:CLASS  15:CLASS  18:CLASS  19:Atom  21:CLASS  22:CLASS
23:CLASS  30:CLASS
31:Atom  32:Atom  33:Atom  34:Atom  35:Atom  36:Atom  37:CLASS  38:CLASS  39:CLASS
40:Atom  41:Atom
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55:CLASS




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FILE LAST UPDATED: 22 Jun 2008  (20080622/ED)

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'OBI' IS DEFAULT SEARCH FIELD FOR 'ZCAPLUS' FILE

=> d stat que L99
L5              STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -  AVAILABLE VIA OFFLINE PRINT *
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Structure attributes must be viewed using STN Express query preparation.
L7          427 SEA FILE=REGISTRY SSS FUL L5
L9          116 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  L7
L83         182 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  CHEON H?/AU
L84        3187 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  YOO S?/AU
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L97       30435 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  LEE K?/AU
L98       68175 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  KIM J?/AU
L99           6 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  (L83 OR L84 OR L85 OR L86 OR
                L87 OR L88 OR L89 OR L90 OR L91 OR L92 OR L93 OR L94 OR L95 OR
                L96 OR L97 OR L98) AND L9


=> s L99 and  L54-L76,L78-L79
L100          6 L99 AND  (L54 OR L55 OR L56 OR L57 OR L58 OR L59 OR L60 OR L61
                OR L62 OR L63 OR L64 OR L65 OR L66 OR L67 OR L68 OR L69 OR L70
                OR L71 OR L72 OR L73 OR L74 OR L75 OR L76 OR L78 OR L79)

=> s L99 or L100
L101          6 L99 OR L100

=> d ibib abs hitind hitstr L101 1-6

L101 ANSWER 1 OF 6  ZCAPLUS  COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER:         2007:1003900  ZCAPLUS  Full-text
DOCUMENT NUMBER:          147:445050
TITLE:                    Apoptotic action of peroxisome proliferator-
                          activated receptor-γ activation in human
                          non-small-cell lung cancer is mediated via proline
                          oxidase-induced reactive oxygen species formation
AUTHOR(S):                Kim, Ki Young; Ahn, Jin Hee; Cheon, Ryae Gyeong
CORPORATE SOURCE:         Center for Metabolic Syndrome Therapeutics, Drug
                          Discovery Division, Korea Research Institute of
                          Chemical Technology, Daejeon, S. Korea
SOURCE:                   Molecular Pharmacology (2007), 72(3), 674-685
                          CODEN: MOPMA3; ISSN: 0026-895X
PUBLISHER:                American Society for Pharmacology and Experimental
                          Therapeutics
DOCUMENT TYPE:            Journal
LANGUAGE:                 English
AB    Peroxisome proliferator-activated receptor (PPAR)-γ ligands have been shown to
      inhibit human lung cancers by inducing apoptosis and differentiation.  In the
      present study, we elucidated the apoptotic mechanism of PPARγ activation in
      human lung cancers by using a novel PPARγ agonist, 1-(trans-methyl-imino-N-
      oxy)-6-(2- morpholinoethoxy)-3-phenyl-1H-i ndene-2-carboxylic acid Et ester
      (KR-62980), and rosiglitazone.  PPARγ activation selectively inhibited cell
      viability of non-small-cell lung cancer with little effect on small-cell lung
```

cancer and normal lung cells. The cell death induced by PPARγ activation presented apoptotic features of oligonucleosomal DNA fragmentation in A549 human non-small-cell lung cancer cell line. Reactive oxygen species (ROS) production was accompanied by increased expression of proline oxidase (POX), a redox enzyme expressed in mitochondria, upon incubation with the agonists. POX RNA interference treatment blocked PPARγ-induced ROS formation and cytotoxicity, suggesting that POX plays a functional role in apoptosis through ROS formation. The apoptotic effects by the agonists were antagonized by bisphenol A diglycidyl ether, a PPARγ antagonist, and by knockdown of PPARγ expression, indicating the involvement of PPARγ in these actions. The results of the present study suggest that PPARγ activation induces apoptotic cell death in non-small-cell lung carcinoma mainly through ROS formation via POX induction.

CC 14-1 (Mammalian Pathological Biochemistry)
Section cross-reference(s): 1

ST PPARgamma proline oxidase reactive oxygen lung carcinoma

IT Apoptosis
Cell differentiation
Cytotoxicity
DNA fragmentation
Human
Mitochondria
(apoptotic action of peroxisome proliferator-activated receptor-γ activation in human non-small-cell lung cancer is mediated via proline oxidase-induced reactive oxygen species formation)

IT Reactive oxygen species
RL: ADV (Adverse effect, including toxicity); BSU (Biological study, unclassified); BIOL (Biological study)
(apoptotic action of peroxisome proliferator-activated receptor-γ activation in human non-small-cell lung cancer is mediated via proline oxidase-induced reactive oxygen species formation)

IT Cytotoxic agents
(effects of KR-62980 and rosiglitazone on cell viability and DNA fragmentation in PPARγ knockdown A549 cells)

IT Cell proliferation
(inhibition; apoptotic action of peroxisome proliferator-activated receptor-γ activation in human non-small-cell lung cancer is mediated via proline oxidase-induced reactive oxygen species formation)

IT Lung, neoplasm
(non-small-cell carcinoma; apoptotic action of peroxisome proliferator-activated receptor-γ activation in human non-small-cell lung cancer is mediated via proline oxidase-induced reactive oxygen species formation)

IT Carcinoma
(pulmonary non-small-cell; apoptotic action of peroxisome proliferator-activated receptor-γ activation in human non-small-cell lung cancer is mediated via proline oxidase-induced reactive oxygen species formation)

IT Peroxisome proliferator-activated receptors
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(γ; apoptotic action of peroxisome proliferator-activated receptor-γ activation in human non-small-cell lung cancer is mediated via proline oxidase-induced reactive oxygen species formation)

IT 7782-44-7D, Oxygen, reactive species, biological studies

RL: ADV (Adverse effect, including toxicity); BSU (Biological study, unclassified); BIOL (Biological study)
(apoptotic action of peroxisome proliferator-activated receptor-γ activation in human non-small-cell lung cancer is mediated via proline oxidase-induced reactive oxygen species formation)

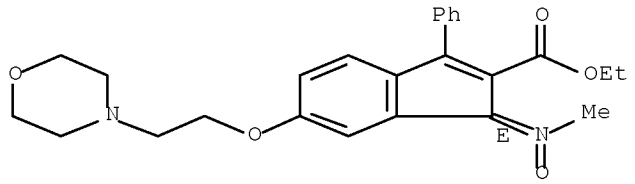
IT 9007-43-6, Cytochrome c, biological studies 9029-17-8, Proline oxidase
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(apoptotic action of peroxisome proliferator-activated receptor-γ activation in human non-small-cell lung cancer is mediated via proline oxidase-induced reactive oxygen species formation)

IT 122320-73-4, Rosiglitazone 867187-61-9, KR-62980
RL: BUU (Biological use, unclassified); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(effects of KR-62980 and rosiglitazone on cell viability and DNA fragmentation in PPARγ knockdown A549 cells)

IT 867187-61-9, KR-62980
RL: BUU (Biological use, unclassified); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(effects of KR-62980 and rosiglitazone on cell viability and DNA fragmentation in PPARγ knockdown A549 cells)

RN 867187-61-9 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-(methyloxidoimino)-6-[2-(4-morpholinyl)ethoxy]-3-phenyl-, ethyl ester, (1E)- (CA INDEX NAME)

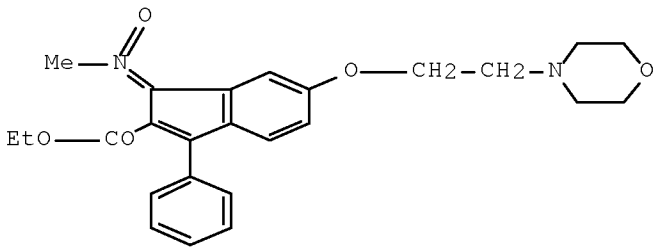
Double bond geometry as shown.



REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L101 ANSWER 2 OF 6 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2007:923593 ZCAPLUS Full-text
DOCUMENT NUMBER: 147:356366
TITLE: Synthesis and structure-activity relationship of novel indene N-oxide derivatives as potent peroxisome proliferator activated receptor γ (PPARγ) agonists
AUTHOR(S): Ahn, Jin Hee; Shin, Mi Sik; Jung, Sun Ho; Kim, Jin Ah; Kim, Hye Min; Kim, Se Hoan; Kang, Seung Kyu; Kim, Kwang Rok; Rhee, Sang Dal; Park, Sung Dae; Lee, Jae Mok; Lee, Jeong Hyung; Cheon, Hyae Gyeong; Kim, Sung Soo
CORPORATE SOURCE: Bioorganic Science Division, Korea Research Institute of Chemical Technology, Daejeon, 305-600, S. Korea
SOURCE: Bioorganic & Medicinal Chemistry Letters (2007), 17(18), 5239-5244
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier Ltd.

DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 147:356366
GI



I

AB A series of novel indene N-oxide derivs. were prepared by various synthetic methods and evaluated for their ability to activate PPARγ. The best PPARγ agonist in this series was 9h (I), which showed an EC50 value of 15 nM.

CC 1-3 (Pharmacology)
Section cross-reference(s): 25

IT Antidiabetic agents
Diabetes mellitus
Structure-activity relationship
(indene N-oxide derivs. as PPARγ agonists)

IT Peroxisome proliferator-activated receptors
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(γ; indene N-oxide derivs. as PPARγ agonists)

IT 867215-17-6P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(indene N-oxide derivs. as PPARγ agonists)

IT 867187-55-1P 867187-61-9P 867187-67-5P
867187-96-0P 867187-98-2P 867188-00-9P
867188-01-0P 867188-05-4P 867188-06-5P
867188-18-9P 867188-20-3P 867188-29-2P
867188-31-6P 867188-42-9P 867188-49-6P
867188-51-0P 867188-53-2P 867188-55-4P
867188-58-7P 867188-60-1P 867188-65-6P 867188-69-0P
867188-73-6P 867188-76-9P 867188-80-5P
949593-50-4P 949593-52-6P 949593-53-7P
949593-62-8P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(indene N-oxide derivs. as PPARγ agonists)

IT 74-88-4, Methyl iodide, reactions 74-96-4, Bromoethane 75-31-0, Isopropyl amine, reactions 97-96-1 100-39-0, Benzyl bromide 100-52-7, Benzaldehyde, reactions 104-87-0 104-88-1, reactions 105-58-8, Diethyl carbonate 120-57-0, 1,3-Benzodioxole-5-carboxaldehyde 123-38-6, Propanal, reactions 498-60-2, 3-Furancarboxaldehyde

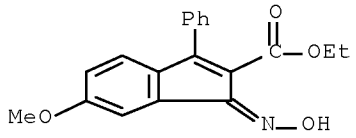
498-62-4, 3-Thiophenecarboxaldehyde 593-77-1, n-Methyl hydroxylamine 620-23-5 765-30-0, Cyclopropyl amine 7803-49-8, Hydroxylamine, reactions 10111-08-7, 1H-Imidazole-2-carboxaldehyde 34068-01-4 850209-49-3 867187-58-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(indene N-oxide derivs. as PPARγ agonists)

IT 73083-19-9P 150356-53-9P 867187-59-5P 867187-62-0P 867187-68-6P 867187-69-7P 867187-70-0P 867187-71-1P 867187-72-2P 867215-03-0P 867215-20-1P 949593-63-9P 949593-64-0P 949593-65-1P 949593-66-2P 949593-67-3P 949593-68-4P 949593-69-5P 949593-70-8P 949593-71-9P 949593-72-0P 949593-73-1P 949593-74-2P 949593-75-3P 949593-76-4P 949593-77-5P 949593-79-7P 949593-81-1P 949593-82-2P 949593-83-3P 949593-85-5P 949593-86-6P 949593-88-8P 949593-90-2P 949593-92-4P 949593-94-6P 949593-96-8P 949593-98-0P 949594-00-7P 949594-02-9P 949594-04-1P 949594-06-3P 949594-08-5P 949594-11-0P 949594-13-2P 949594-15-4P 949594-17-6P 949594-19-8P 949594-21-2P 949594-23-4P 949594-25-6P 949594-26-7P 949594-27-8P 949594-28-9P 949594-29-0P 949594-30-3P 949594-31-4P 949594-32-5P 949594-33-6P 949594-34-7P 949594-35-8P 949594-36-9P 949594-37-0P 949594-38-1P 949594-39-2P 949594-40-5P 949594-41-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(indene N-oxide derivs. as PPARγ agonists)

IT 1005136-47-9P 1005137-04-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(indene N-oxide derivs. as PPARγ agonists)

IT 867215-17-6P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(indene N-oxide derivs. as PPARγ agonists)

RN 867215-17-6 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-(hydroxyimino)-6-methoxy-3-phenyl-, ethyl ester (CA INDEX NAME)

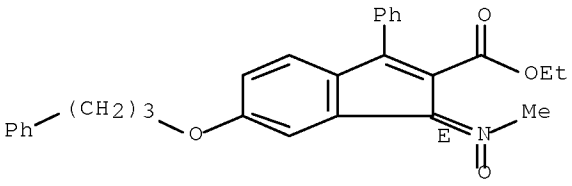


IT 867187-55-1P 867187-61-9P 867187-67-5P 867187-96-0P 867187-98-2P 867188-00-9P 867188-01-0P 867188-05-4P 867188-18-9P 867188-20-3P 867188-29-2P 867188-31-6P 867188-42-9P 867188-49-6P 867188-51-0P 867188-53-2P 867188-55-4P 867188-69-0P 867188-76-9P 867188-80-5P 949593-50-4P 949593-52-6P 949593-62-8P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(indene N-oxide derivs. as PPARγ agonists)

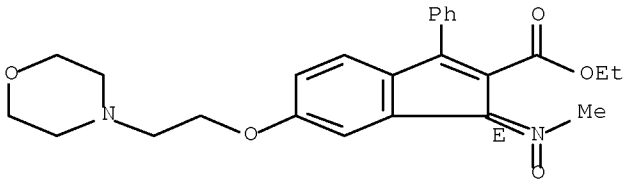
RN 867187-55-1 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-(methyloxidoimino)-3-phenyl-6-(3-phenylpropoxy)-, ethyl ester, (1E)- (CA INDEX NAME)

Double bond geometry as shown.



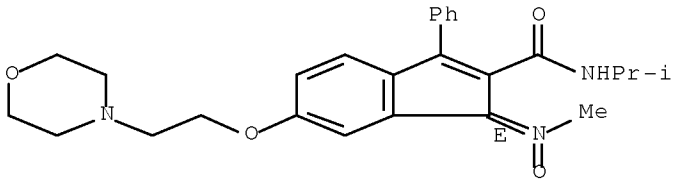
RN 867187-61-9 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-(methyloxidoimino)-6-[2-(4-morpholinyl)ethoxy]-3-phenyl-, ethyl ester, (1E)- (CA INDEX NAME)

Double bond geometry as shown.



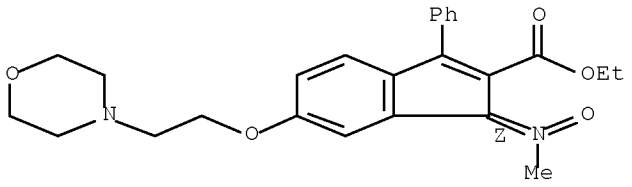
RN 867187-67-5 ZCAPLUS
CN 1H-Indene-2-carboxamide, N-(1-methylethyl)-1-(methyloxidoimino)-6-[2-(4-morpholinyl)ethoxy]-3-phenyl-, (1E)- (CA INDEX NAME)

Double bond geometry as shown.



RN 867187-96-0 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-(methyloxidoimino)-6-[2-(4-morpholinyl)ethoxy]-3-phenyl-, ethyl ester, (1Z)- (CA INDEX NAME)

Double bond geometry as shown.



RN 867187-98-2 ZCAPLUS
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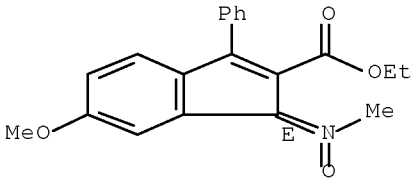
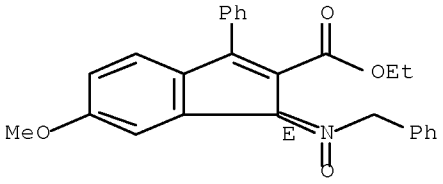
Double bond geometry as shown.



RN 867188-00-9 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 6-methoxy-1-[oxido(phenylmethyl)imino]-3-phenyl-, ethyl ester, (1E)- (CA INDEX NAME)

Double bond geometry as shown.



RN 867188-01-0 ZCAPLUS
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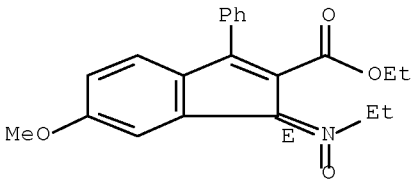
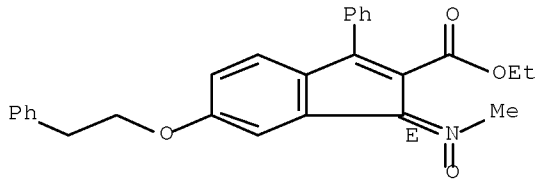
Double bond geometry as shown.



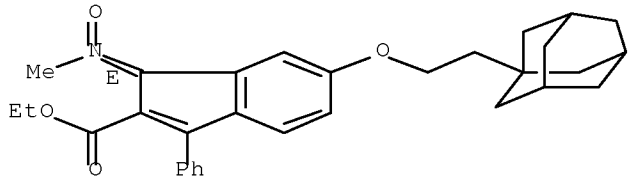
RN 867188-05-4 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-(methyloxidoimino)-3-phenyl-6-(2-phenylethoxy)-, ethyl ester, (1E)- (CA INDEX NAME)

Double bond geometry as shown.



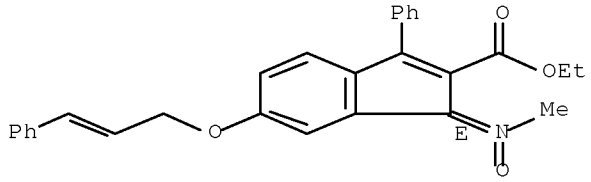
RN 867188-18-9 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-(methyloxidoimino)-3-phenyl-6-(2-tricyclo[3.3.1.13,7]dec-1-ylethoxy)-, ethyl ester, (1E)- (CA INDEX NAME)

Double bond geometry as shown.



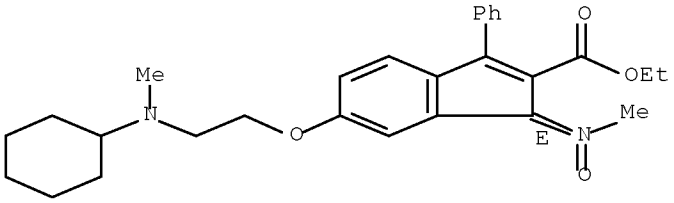
RN 867188-20-3 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-(methyloxidoimino)-3-phenyl-6-[(3-phenyl-2-propen-1-yl)oxy]-, ethyl ester, (1E)- (CA INDEX NAME)

Double bond geometry as described by E or Z.



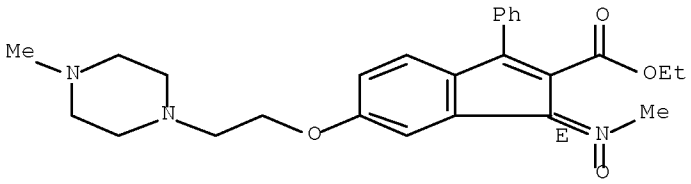
RN 867188-29-2 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 6-[2-(cyclohexylmethylamino)ethoxy]-1-(methyloxidoimino)-3-phenyl-, ethyl ester, (1E)- (CA INDEX NAME)

Double bond geometry as shown.



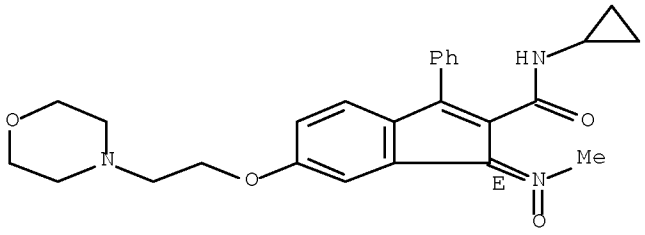
RN 867188-31-6 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-(methyloxidoimino)-6-[2-(4-methyl-1-piperazinyl)ethoxy]-3-phenyl-, ethyl ester, (1E)- (CA INDEX NAME)

Double bond geometry as shown.



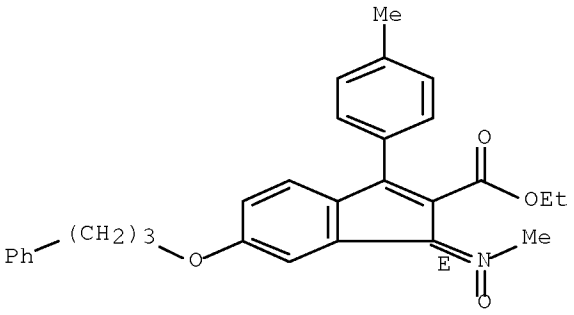
RN 867188-42-9 ZCAPLUS
CN 1H-Indene-2-carboxamide, N-cyclopropyl-1-(methyloxidoimino)-6-[2-(4-morpholinyl)ethoxy]-3-phenyl-, (1E)- (CA INDEX NAME)

Double bond geometry as shown.



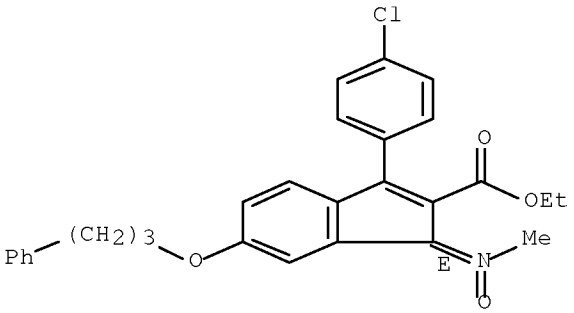
RN 867188-49-6 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-(methyloxidoimino)-3-(4-methylphenyl)-6-(3-phenylpropoxy)-, ethyl ester, (1E)- (CA INDEX NAME)

Double bond geometry as shown.



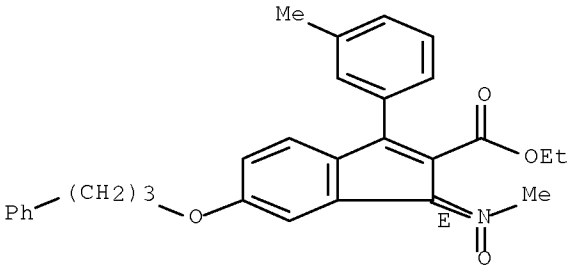
RN 867188-51-0 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 3-(4-chlorophenyl)-1-(methyloxidoimino)-6-(3-phenylpropoxy)-, ethyl ester, (1E)- (CA INDEX NAME)

Double bond geometry as shown.



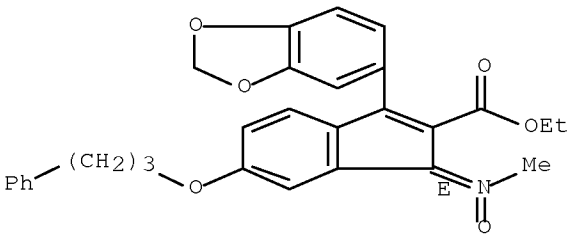
RN 867188-53-2 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-(methyloxidoimino)-3-(3-methylphenyl)-6-(3-phenylpropoxy)-, ethyl ester, (1E)- (CA INDEX NAME)

Double bond geometry as shown.



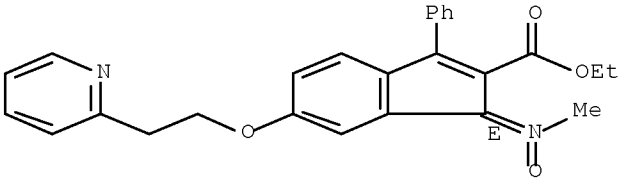
RN 867188-55-4 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 3-(1,3-benzodioxol-5-yl)-1-(methyloxidoimino)-6-(3-phenylpropoxy)-, ethyl ester, (1E)- (CA INDEX NAME)

Double bond geometry as shown.



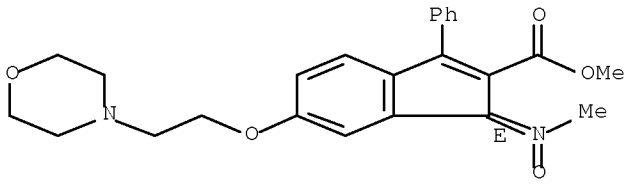
RN 867188-69-0 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-(methyloxidoimino)-3-phenyl-6-[2-(2-pyridinyl)ethoxy]-, ethyl ester, (1E)- (CA INDEX NAME)

Double bond geometry as shown.



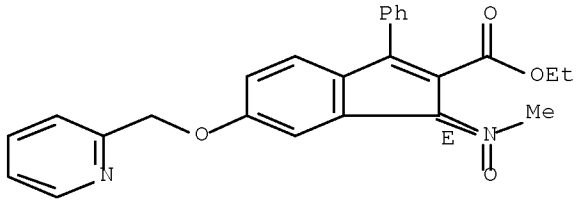
RN 867188-76-9 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-(methyloxidoimino)-6-[2-(4-morpholinyl)ethoxy]-3-phenyl-, methyl ester, (1E)- (CA INDEX NAME)

Double bond geometry as shown.

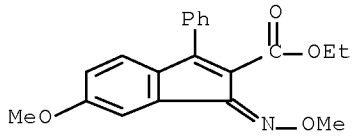


RN 867188-80-5 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-(methyloxidoimino)-3-phenyl-6-(2-pyridinylmethoxy)-, ethyl ester, (1E)- (CA INDEX NAME)

Double bond geometry as shown.

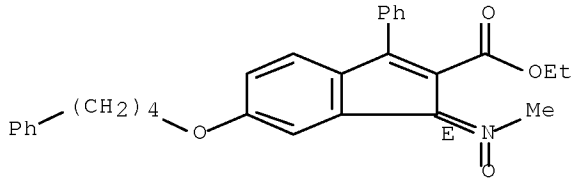


RN 949593-50-4 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 6-methoxy-1-(methoxyimino)-3-phenyl-, ethyl ester (CA INDEX NAME)



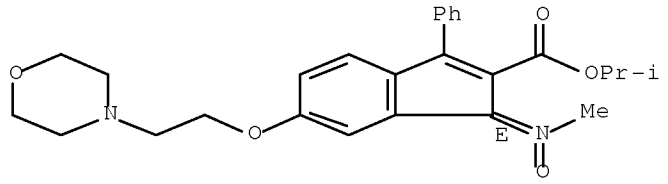
RN 949593-52-6 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-(methyloxidoimino)-3-phenyl-6-(4-phenylbutoxy)-, ethyl ester, (1E)- (CA INDEX NAME)

Double bond geometry as shown.



RN 949593-62-8 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-(methyloxidoimino)-6-[2-(4-morpholinyl)ethoxy]-3-phenyl-, 1-methylethyl ester, (1E)- (CA INDEX NAME)

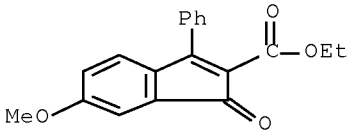
Double bond geometry as shown.



IT 850209-49-3

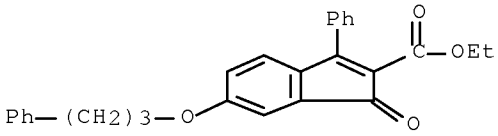
RL: RCT (Reactant); RACT (Reactant or reagent)
(indene N-oxide derivs. as PPARγ agonists)

RN 850209-49-3 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 6-methoxy-1-oxo-3-phenyl-, ethyl ester (CA INDEX NAME)

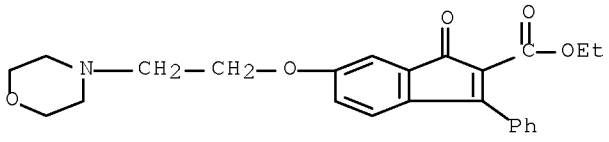


IT 867187-59-5P 867187-62-0P 867187-72-2P
867215-03-0P 949593-63-9P 949593-64-0P
949593-65-1P 949593-66-2P 949593-67-3P
949593-68-4P 949593-69-5P 949594-35-8P
949594-36-9P 949594-37-0P 949594-38-1P
949594-39-2P 949594-40-5P 949594-41-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(indene N-oxide derivs. as PPARγ agonists)

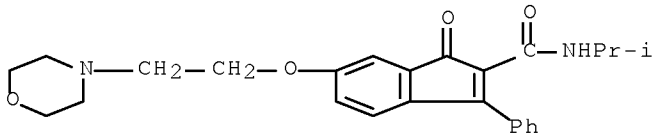
RN 867187-59-5 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-oxo-3-phenyl-6-(3-phenylpropoxy)-, ethyl ester (CA INDEX NAME)



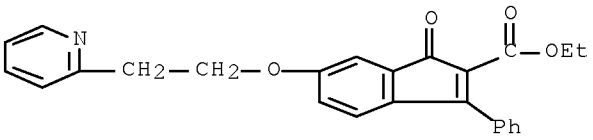
RN 867187-62-0 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 6-[2-(4-morpholinyl)ethoxy]-1-oxo-3-phenyl-, ethyl ester (CA INDEX NAME)



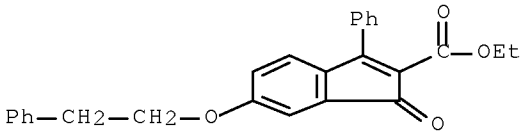
RN 867187-72-2 ZCAPLUS
CN 1H-Indene-2-carboxamide, N-(1-methylethyl)-6-[2-(4-morpholinyl)ethoxy]-1-oxo-3-phenyl- (CA INDEX NAME)



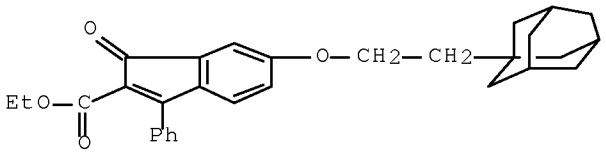
RN 867215-03-0 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-oxo-3-phenyl-6-[2-(2-pyridinyl)ethoxy]-, ethyl ester (CA INDEX NAME)



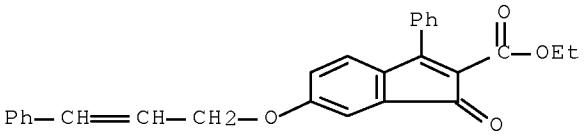
RN 949593-63-9 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-oxo-3-phenyl-6-(2-phenylethoxy)-, ethyl ester (CA INDEX NAME)



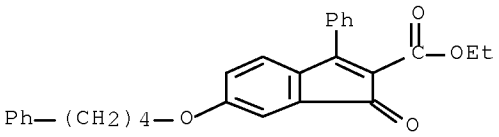
RN 949593-64-0 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-oxo-3-phenyl-6-(2-tricyclo[3.3.1.13,7]dec-1-ylethoxy)-, ethyl ester (CA INDEX NAME)



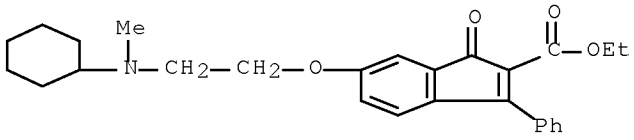
RN 949593-65-1 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-oxo-3-phenyl-6-[(3-phenyl-2-propen-1-yl)oxy]-, ethyl ester (CA INDEX NAME)



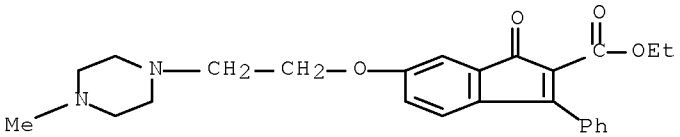
RN 949593-66-2 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-oxo-3-phenyl-6-(4-phenylbutoxy)-, ethyl ester (CA INDEX NAME)



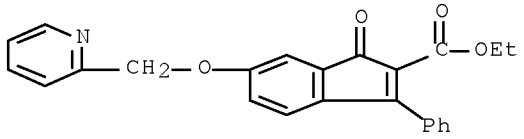
RN 949593-67-3 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 6-[2-(cyclohexylmethylamino)ethoxy]-1-oxo-3-phenyl-, ethyl ester (CA INDEX NAME)



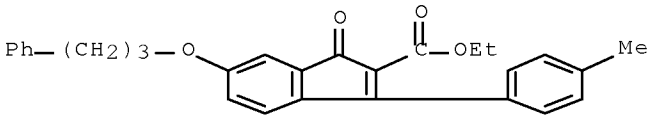
RN 949593-68-4 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 6-[2-(4-methyl-1-piperazinyl)ethoxy]-1-oxo-3-phenyl-, ethyl ester (CA INDEX NAME)



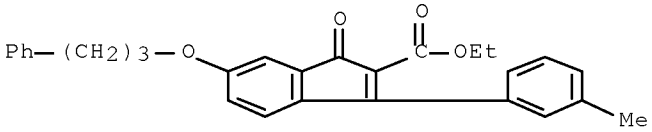
RN 949593-69-5 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-oxo-3-phenyl-6-(2-pyridinylmethoxy)-, ethyl ester (CA INDEX NAME)



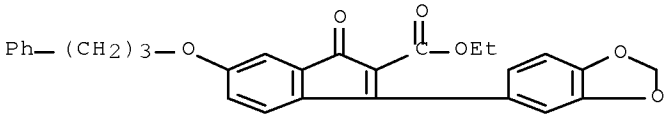
RN 949594-35-8 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 3-(4-methylphenyl)-1-oxo-6-(3-phenylpropoxy)-, ethyl ester (CA INDEX NAME)



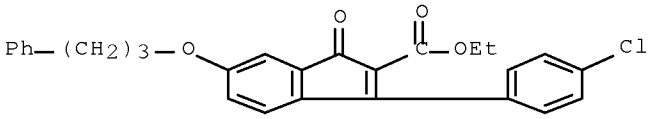
RN 949594-36-9 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 3-(3-methylphenyl)-1-oxo-6-(3-phenylpropoxy)-, ethyl ester (CA INDEX NAME)



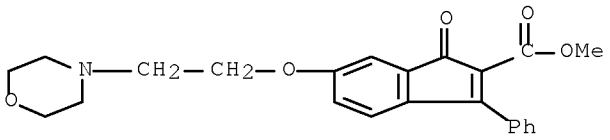
RN 949594-37-0 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 3-(1,3-benzodioxol-5-yl)-1-oxo-6-(3-phenylpropoxy)-, ethyl ester (CA INDEX NAME)



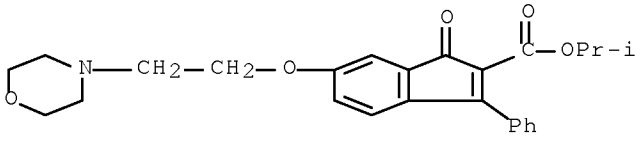
RN 949594-38-1 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 3-(4-chlorophenyl)-1-oxo-6-(3-phenylpropoxy)-, ethyl ester (CA INDEX NAME)



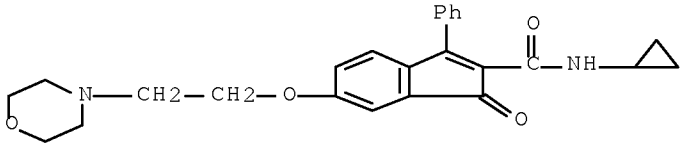
RN 949594-39-2 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 6-[2-(4-morpholinyl)ethoxy]-1-oxo-3-phenyl-, methyl ester (CA INDEX NAME)



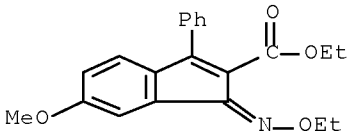
RN 949594-40-5 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 6-[2-(4-morpholinyl)ethoxy]-1-oxo-3-phenyl-, 1-methylethyl ester (CA INDEX NAME)



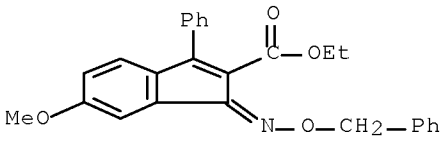
RN 949594-41-6 ZCAPLUS
CN 1H-Indene-2-carboxamide, N-cyclopropyl-6-[2-(4-morpholinyl)ethoxy]-1-oxo-3-phenyl- (CA INDEX NAME)



IT 1005136-47-9P 1005137-04-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(indene N-oxide derivs. as PPARγ agonists)
RN 1005136-47-9 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-(ethoxyimino)-6-methoxy-3-phenyl-, ethyl ester (CA INDEX NAME)



RN 1005137-04-1 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 6-methoxy-3-phenyl-1-[(phenylmethoxy)imino]-, ethyl ester (CA INDEX NAME)



REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L101 ANSWER 3 OF 6 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2006:822209 ZCAPLUS Full-text
DOCUMENT NUMBER: 145:410197
TITLE: Differential anti-proliferative actions of peroxisome proliferator-activated receptor-γ agonists in MCF-7 breast cancer cells
AUTHOR(S): Kim, Ki Young; Kim, Sung Soo; Cheon, Hyae Gyeong
CORPORATE SOURCE: Bioorganic Science Division, Korea Research Institute of Chemical Technology, Daejeon, 305-600, S. Korea
SOURCE: Biochemical Pharmacology (2006), 72(5), 530-540
CODEN: BCPCA6; ISSN: 0006-2952
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Peroxisome proliferator-activated receptor-γ (PPARγ) activation has been a new approach to cancer therapy. In the present study, we investigated the effects of two structurally different PPARγ agonists, rosiglitazone and KR-62980 on MCF-7 breast cancer cells. Both agonists inhibited the cell proliferation and colony formation via apoptosis. PTEN expression was increased with decreased Akt phosphorylation by the agonists, whereas agonists actions were abolished in PTEN knockdown cells, indicating the critical role of PTEN in the anti-proliferative effects of PPARγ activation. Rosiglitazone induced the MCF-7 cell differentiation but KR-62980 did not alter the differentiation pattern with little effects on the lipid accumulation and the expression of lipogenesis markers. These results suggest that PPARγ activation may result in the inhibition of cell proliferation and/or induction of cell differentiation depending on the type of PPARγ agonists, and that KR-62980 may be useful in breast cancer therapy by inducing apoptosis.

CC 1-6 (Pharmacology)
ST PPAR gamma agonist breast cancer
IT Antitumor agents
Human

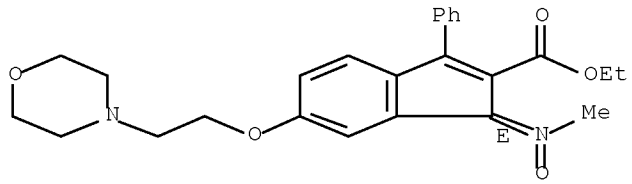
Mammary gland, neoplasm
(differential anti-proliferative actions of peroxisome proliferator-activated receptor-γ agonists in MCF-7 breast cancer cells)

IT 122320-73-4, Rosiglitazone 867187-61-9, KR 62980
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(differential anti-proliferative actions of peroxisome proliferator-activated receptor-γ agonists in MCF-7 breast cancer cells)

IT 867187-61-9, KR 62980
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(differential anti-proliferative actions of peroxisome proliferator-activated receptor-γ agonists in MCF-7 breast cancer cells)

RN 867187-61-9 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-(methyloxidoimino)-6-[2-(4-morpholinyl)ethoxy]-3-phenyl-, ethyl ester, (1E)- (CA INDEX NAME)

Double bond geometry as shown.



REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L101 ANSWER 4 OF 6 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2006:711783 ZCAPLUS Full-text
DOCUMENT NUMBER: 145:328107
TITLE: KR-62980: A novel peroxisome proliferator-activated receptor γ agonist with weak adipogenic effects
AUTHOR(S): Kim, Kwang Rok; Lee, Jeong Hyung; Kim, Seung Jun; Rhee, Sang Dal; Jung, Won Hoon; Yang, Sung-Don; Kim, Sung Soo; Ahn, Jin Hee; Cheon, Hyae Gyeong
CORPORATE SOURCE: Medicinal Science Division, Korea Research Institute of Chemical Technology, Daejeon, Yuseong-Gu, 305-343, S. Korea
SOURCE: Biochemical Pharmacology (2006), 72(4), 446-454
CODEN: BCPCA6; ISSN: 0006-2952
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The nuclear receptor peroxisome proliferator-activated receptor γ (PPARγ) is the target for the anti-diabetic drugs including thiazolidinediones. We report here the identification and characterization of a novel PPARγ agonist KR-62980. KR-62980 acted as a selective PPARγ agonist in transactivation assay with an EC50 of 15 nM. In fully differentiated 3T3-L1 adipocytes, KR-62980 induced [3H]-deoxyglucose uptake in a concentration-dependent manner in

the presence of insulin. KR-62980 was weakly adipogenic with little induction of aP2 mRNA, and was able to antagonize the adipogenic effects of rosiglitazone in C3H10T1/2 cells. In vivo pharmacokinetic profile of KR-62980 revealed that the compound exhibited good oral bioavailability of 65% with a terminal elimination half-life of 2.5 h in the rat. Treatment of high fat diet-induced C57BL/6J mice with KR-62980 for 14 days reduced plasma glucose levels with little side effects with regard to weight gain, cardiac hypertrophy and hepatotoxicity. These results suggest that KR-62980 acts as a selective PPARγ modulator with anti-hyperglycemic activity, and that the mechanism of actions of KR-62980 appears to be different from that of rosiglitazone with improved side effect profiles.

CC 1-10 (Pharmacology)

ST KR62980 peroxisome proliferator activated receptor gamma weak adipogenic

IT Antidiabetic agents
Diabetes mellitus
Hepatotoxicity
(KR-62980 is a novel peroxisome proliferator-activated receptor γ agonist with weak adipogenic effects)

IT Adipose tissue
(adipocyte; KR-62980 is a novel peroxisome proliferator-activated receptor γ agonist with weak adipogenic effects)

IT Hypertrophy
(cardiac; KR-62980 is a novel peroxisome proliferator-activated receptor γ agonist with weak adipogenic effects)

IT Cytoprotective agents
(hepatoprotective agents; KR-62980 is a novel peroxisome proliferator-activated receptor γ agonist with weak adipogenic effects)

IT Heart, disease
(hypertrophy; KR-62980 is a novel peroxisome proliferator-activated receptor γ agonist with weak adipogenic effects)

IT Peroxisome proliferator-activated receptors
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(γ; KR-62980 is a novel peroxisome proliferator-activated receptor γ agonist with weak adipogenic effects)

IT 9004-10-8, Insulin, biological studies
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(KR-62980 is a novel peroxisome proliferator-activated receptor γ agonist with weak adipogenic effects)

IT 867187-61-9, KR 62980
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(KR-62980 is a novel peroxisome proliferator-activated receptor γ agonist with weak adipogenic effects)

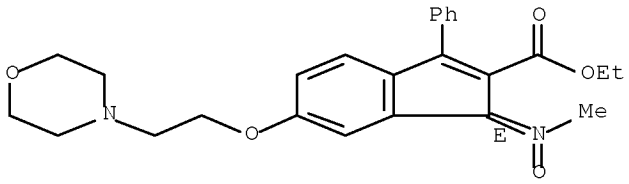
IT 50-99-7, D-Glucose, biological studies
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(blood; KR-62980 is a novel peroxisome proliferator-activated receptor γ agonist with weak adipogenic effects)

IT 867187-61-9, KR 62980
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(KR-62980 is a novel peroxisome proliferator-activated receptor γ agonist with weak adipogenic effects)

RN 867187-61-9 ZCAPLUS

CN 1H-Indene-2-carboxylic acid, 1-(methyloxidoimino)-6-[2-(4-morpholinyl)ethoxy]-3-phenyl-, ethyl ester, (1E)- (CA INDEX NAME)

Double bond geometry as shown.



REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L101 ANSWER 5 OF 6 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2006:643683 ZCAPLUS Full-text
DOCUMENT NUMBER: 145:240947
TITLE: Indenone Derivatives: A Novel Template for Peroxisome Proliferator-Activated Receptor γ (PPARγ) Agonists
AUTHOR(S): Ahn, Jin Hee; Shin, Mi Sik; Jung, Sun Ho; Kang, Seung Kyu; Kim, Kwang Rok; Rhee, Sang Dal; Jung, Won Hoon; Yang, Sung Don; Kim, Seung Jun; Woo, Joo Rang; Lee, Jeong Hyung; Cheon, Hyae Gyeong; Kim, Sung Soo
CORPORATE SOURCE: Bioorganic Science Division, Korea Research Institute of Chemical Technology, Daejeon, 305-600, S. Korea
SOURCE: Journal of Medicinal Chemistry (2006), 49(15), 4781-4784
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 145:240947

AB Agonists of peroxisome proliferator-activated receptor γ (PPAR γ) are of interest as a treatment for diabetes, which prompted the identification of a new class of non-TZD PPAR γ agonist. Moreover, one compound has displayed the most active agonistic activity with an EC50 value of 50 nM, in addition to exhibiting a new binding mode in the x-ray cocrystal structure.

CC 1-3 (Pharmacology)
ST indenone deriv peroxisome proliferator receptor gamma
IT Antidiabetic agents
Crystal structure
Diabetes mellitus
Molecular modeling
Structure-activity relationship
(indenone derivs.: a novel template for peroxisome proliferator-activated receptor γ (PPARγ) agonists)
IT Polyphosphoric acids
RL: RGT (Reagent); RACT (Reactant or reagent)
(indenone derivs.: a novel template for peroxisome proliferator-activated receptor γ (PPARγ) agonists)
IT Peroxisome proliferator-activated receptors
RL: BSU (Biological study, unclassified); BIOL (Biological study)

(γ; indenone derivs.: a novel template for peroxisome proliferator-activated receptor γ (PPARγ) agonists)

IT 123-91-1, 1,4-Dioxane, uses
RL: NUU (Other use, unclassified); USES (Uses)
(indenone derivs.: a novel template for peroxisome proliferator-activated receptor γ (PPARγ) agonists)

IT 850209-49-3P, 6-Methoxy-1-oxo-3-phenyl-1H-indene-2-carboxylic Acid Ethyl Ester 867214-90-2P, 6-Methoxy-3-phenyl-1H-indene-2-carboxylic Acid Ethyl Ester
RL: PAC (Pharmacological activity); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(indenone derivs.: a novel template for peroxisome proliferator-activated receptor γ (PPARγ) agonists)

IT 867187-59-5P, 1-Oxo-3-phenyl-6-(3-phenylpropoxy)-1H-indene-2-carboxylic acid Ethyl Ester 867215-17-6P, 1-Hydroxyimino-6-Methoxy-3-phenyl-1H-indene-2-carboxylic Acid Ethyl Ester 906369-99-1P 906370-00-1P 906370-01-2P 906370-02-3P 906370-03-4P
RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(indenone derivs.: a novel template for peroxisome proliferator-activated receptor γ (PPARγ) agonists)

IT 867187-56-2P, 2-(3-Hydroxybenzyl)-3-oxo-3-phenylpropionic acid ethyl ester 867187-57-3P, 6-Hydroxy-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867214-92-4P, 2-(3-Methoxybenzyl)-3-oxo-3-phenylpropionic acid ethyl ester
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(indenone derivs.: a novel template for peroxisome proliferator-activated receptor γ (PPARγ) agonists)

IT 94-02-0, Ethyl benzoylacetate 100-39-0, Benzyl bromide 103-63-9 123-25-1, Diethyl succinate 611-94-9, 4-Methoxybenzophenone 637-59-2, 1-Bromo-3-phenylpropane 824-98-6, 3-Methoxybenzyl chloride 19386-06-2 36878-91-8 60760-06-7, 3-Chloromethylphenol
RL: RCT (Reactant); RACT (Reactant or reagent)
(indenone derivs.: a novel template for peroxisome proliferator-activated receptor γ (PPARγ) agonists)

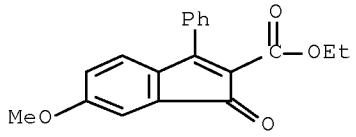
IT 101736-96-3P 109309-43-5P 110050-42-5P 132725-35-0P 860222-57-7P 867187-58-4P 916793-00-5P 916793-01-6P 916793-11-8P 916793-13-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(indenone derivs.: a novel template for peroxisome proliferator-activated receptor γ (PPARγ) agonists)

IT 7446-08-4, Selenium oxide (SeO2)
RL: RGT (Reagent); RACT (Reactant or reagent)
(indenone derivs.: a novel template for peroxisome proliferator-activated receptor γ (PPARγ) agonists)

IT 850209-49-3P, 6-Methoxy-1-oxo-3-phenyl-1H-indene-2-carboxylic Acid Ethyl Ester
RL: PAC (Pharmacological activity); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study);

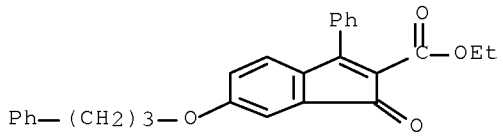
PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(indenone derivs.: a novel template for peroxisome proliferator-activated receptor γ (PPARγ) agonists)

RN 850209-49-3 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 6-methoxy-1-oxo-3-phenyl-, ethyl ester (CA INDEX NAME)

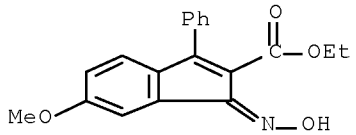


IT 867187-59-5P, 1-Oxo-3-phenyl-6-(3-phenylpropoxy)-1H-indene-2-carboxylic acid Ethyl Ester 867215-17-6P, 1-Hydroxyimino-6-Methoxy-3-phenyl-1H-indene-2-carboxylic Acid Ethyl Ester 906370-02-3P
RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(indenone derivs.: a novel template for peroxisome proliferator-activated receptor γ (PPARγ) agonists)

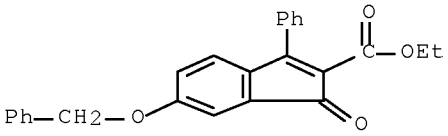
RN 867187-59-5 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-oxo-3-phenyl-6-(3-phenylpropoxy)-, ethyl ester (CA INDEX NAME)



RN 867215-17-6 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-(hydroxyimino)-6-methoxy-3-phenyl-, ethyl ester (CA INDEX NAME)



RN 906370-02-3 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-oxo-3-phenyl-6-(phenylmethoxy)-, ethyl ester (CA INDEX NAME)

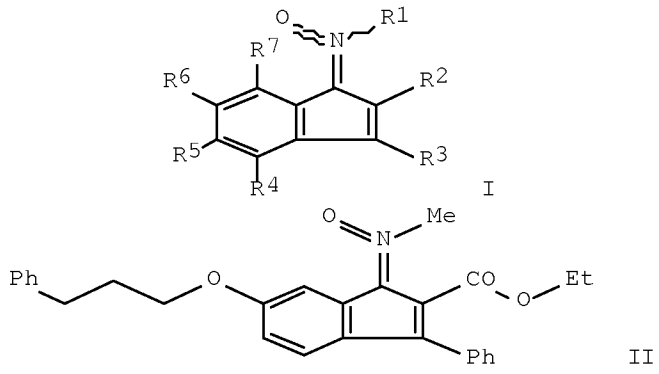


REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L101 ANSWER 6 OF 6 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2005:1154517 ZCAPLUS Full-text
DOCUMENT NUMBER: 143:405637
TITLE: Preparation of 1H-inden-1-imine N-oxides as selective modulators of peroxisome proliferator activated receptors
INVENTOR(S): Cheon, Hyae Gyeong; Yoo, Sung-Eun; Kim, Sung Soo; Yang, Sung-Don; Rhee, Sang Dal; Ahn, Jin Hee; Kang, Seung Kyu; Jung, Won Hoon; Park, Sung Dae; et al.
PATENT ASSIGNEE(S): Korea Research Institute of Chemical Technology, S. Korea; Jeil Pharm. Co., Ltd.; Korea Research Institute of Bioscience and Biotechnology; Cj Corp.; et al.
SOURCE: PCT Int. Appl., 90 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005100303	A1	20051027	WO 2005-KR1066	20050413
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
KR 2005100051	A	20051018	KR 2004-25217	20040413
AU 2005233039	A1	20051027	AU 2005-233039	20050413
AU 2005233039	B2	20080313		
CA 2563000	A1	20051027	CA 2005-2563000	20050413
EP 1740531	A1	20070110	EP 2005-733398	20050413
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR				
CN 1942434	A	20070404	CN 2005-80011181	20050413
BR 2005009794	A	20071023	BR 2005-9794	20050413
JP 2007532635	T	20071115	JP 2007-508276	20050413
MX 2006PA11513	A	20070704	MX 2006-PA11513	20061005
US 20070185109	A1	20070809	US 2006-599911	20061023

IN 2006DN06487 A 20070831 IN 2006-DN6487 20061102
PRIORITY APPLN. INFO.: KR 2004-25217 A 20040413
WO 2005-KR1066 W 20050413
OTHER SOURCE(S): CASREACT 143:405637; MARPAT 143:405637
GI



I

II

AB The inventive 1H-inden-1-imine N-oxides (shown as I; variables defined below; e.g. 1-(trans-N-methyl-N-oxoimino)-3-phenyl-6-(3-phenylpropoxy)-1H- indene-2-carboxylic acid Et ester (shown as II)) are capable of selectively modulating the activities of peroxisome proliferator activated receptors (PPARs), causing no adverse side effects, and thus, they are useful for the treatment and prevention of disorders modulated by PPARs, i.e., metabolic syndromes such as diabetes, obesity, arteriosclerosis, hyperlipidemia, hyperinsulinism and hypertension, inflammatory diseases such as osteoporosis, liver cirrhosis and asthma, and cancer. For I: R1 is C1-6 alkyl, C1-6 alkenyl or C3-6 cycloalkyl, which is (un)substituted with ≥1 Ph groups; R2 is H, CN, CO2Ra, CH2CO2Ra, CONRbRc, morpholinocarbonyl, thiomorpholinocarbonyl, 4-Rapiperazin-1-ylcarbonyl, or phenyl; R3 is C1-6 alkyl, C3-6 cycloalkyl, or naphthyl, Ph, furanyl, thienyl, benzothienyl or imidazolyl, which is (un)substituted with ≥1 halogen, CN, NH2, NO2, ORa, phenyloxy, C1-6 alkyl and C3-6 cycloalkyl; and R4, R5, R6 and R7 = H, OH, OSO2CH3, O(CH2)mRe, CH2Rf, OCOCH2ORg, OCH2CH2ORg or OCH2CH:CHRg, or R5 and R6 together form OCH2O; in which Ra is H, or C1-6 alkyl or C3-6 cycloalkyl, which is (un)substituted with ≥1 halogens; Rb and Rc = H, C1-6 alkyl or C3-6 cycloalkyl; Rd is O, S or NRa; Re is H, halogen, C3-6 cycloalkyl, naphthyl, Rapyridinyl, morpholinocarbonyl, thiomorpholinocarbonyl, 4-Rapiperazin-1-ylcarbonyl, CyNRa, 2-phenyl-5-Rathiazol-4-yl, 4-RgCH2morpholino or Ph, which is (un)substituted with ≥1 halogen, CN, NH2, NO2, ORa, CF3 and COORa; Rf is OCH2CH2Rg, morpholinocarbonyl, thiomorpholinocarbonyl, 4-Rapiperazin-1-ylcarbonyl; Rg is Ph, which is (un)substituted with ≥1 halogen, CN, NH2, NO2 and ORa; and m = 1-5. Methods of preparation are claimed and 10 example prepns. are included. For example, II was prepared in 6 steps (99, 75, 47, 58, 85, and 40 % yields) starting with preparation of 3-hydroxybenzyl chloride from 3-hydroxybenzyl alc. followed by preparation of intermediates 2-(3-hydroxybenzyl)-3-oxo-3-phenylpropionic acid Et ester, 6-hydroxy-3-phenyl-1H-indene-2-carboxylic acid Et ester, 6-hydroxy-1-oxo-3-phenyl-1H-indene-2-carboxylic acid Et ester, and 3-phenyl-6-(3-phenylpropyloxy)-1-oxo-1H-indene-2-carboxylic acid Et ester. EC50 values for activation of PPARγ are tabulated for 27 examples of I; they exhibited superior activation over rosiglitazone. One example of I was tested for effectiveness in lowering blood glucose level in ob/ob mice; it has an

excellent effect in lowering both blood glucose and insulin levels, when it is administered by either orally or i.p. with no side effects such as weight gain, hepatotoxicity or cardiotoxicity.

IC ICM C07C251-44

CC 24-7 (Alicyclic Compounds)
Section cross-reference(s): 1, 2, 63

ST indenimine oxide prepn selective modulator peroxisome proliferator activated receptor

IT Heart
Liver
(lack of toxicity of potential drug; preparation of 1H-inden-1-imine N-oxides as selective modulators of peroxisome proliferator activated receptors)

IT Cardiotoxicity
Drug toxicity
Hepatotoxicity
(lack of; preparation of 1H-inden-1-imine N-oxides as selective modulators of peroxisome proliferator activated receptors)

IT Peroxisome proliferator-activated receptors
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(modulators; preparation of 1H-inden-1-imine N-oxides as selective modulators of peroxisome proliferator activated receptors)

IT Antiarteriosclerotics
Antiasthmatics
Antidiabetic agents
Antihypertensives
Antiobesity agents
Antitumor agents
Arteriosclerosis
Asthma
Cirrhosis
Diabetes mellitus
Drug delivery systems
Human
Hypertension
Hypolipemic agents
Neoplasm
Obesity
Osteoporosis
(preparation of 1H-inden-1-imine N-oxides as selective modulators of peroxisome proliferator activated receptors)

IT Hyperlipidemia
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(preparation of 1H-inden-1-imine N-oxides as selective modulators of peroxisome proliferator activated receptors)

IT Peroxisome proliferator-activated receptors
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(γ, modulators; preparation of 1H-inden-1-imine N-oxides as selective modulators of peroxisome proliferator activated receptors)

IT 867187-61-9P, 1-(trans-N-Methyl-N-oxoimino)-6-[2-(morpholin-4-yl)ethoxy]-3-phenyl-1H-indene-2-carboxylic acid ethyl ester
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(drug candidate; preparation of 1H-inden-1-imine N-oxides as selective modulators of peroxisome proliferator activated receptors)

IT 867187-55-1P, 1-(trans-N-Methyl-N-oxoimino)-3-phenyl-6-(3-phenylpropoxy)-1H-indene-2-carboxylic acid ethyl ester 867187-63-1P, 1-(trans-N-Methyl-N-oxoimino)-5,6-methylenedioxy-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867187-67-5P, 1-(trans-N-Methyl-N-

oxoimino)-6-[2-(morpholin-4-yl)ethoxy]-3-phenyl-1H-indene-2-carboxylic acid isopropylamide 867187-75-5P, 1-(trans-N-Methyl-N-oxoimino)-3-phenyl-6-(3-phenylpropoxy)-1H-indene-2-carbonitrile 867187-83-5P , 1-(trans-N-Methyl-N-oxoimino)-6-[(morpholin-4-yl)methyl]-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867187-89-1P, 1-(trans-N-Methyl-N-oxoimino)-3-phenyl-6-(3-phenylpropoxy)-1H-indene-2-carboxylic acid cyclohexylamide 867187-93-7P, 1-(trans-N-Methyl-N-oxoimino)-3-phenyl-5-[2-(pyridin-2-yl)ethoxy]-1H-indene-2-carboxylic acid isopropylamide 867187-96-0P, 1-(cis-N-Methyl-N-oxoimino)-6-[2-(morpholin-4-yl)ethoxy]-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867187-98-2P, 6-Methoxy-1-(trans-N-methyl-N-oxoimino)-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867187-99-3P, 1-(trans-N-Isopropyl-N-oxoimino)-6-methoxy-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867188-00-9P, 1-(trans-N-Benzyl-N-oxoimino)-6-methoxy-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867188-01-0P, 1-(trans-N-Ethyl-N-oxoimino)-6-methoxy-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867188-02-1P, 6-Methoxy-1-[trans-N-(3-phenylpropyl)-N-oxoimino]-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867188-03-2P, 6-Methoxy-1-[trans-N-(3-methyl-2-butenyl)-N-oxoimino]-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867188-04-3P, 1-(trans-N-Isobutyl-N-oxoimino)-6-methoxy-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867188-05-4P, 1-(trans-N-Methyl-N-oxoimino)-6-phenethyloxy-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867188-06-5P, 3-(Furan-3-yl)-1-(trans-N-methyl-N-oxoimino)-6-(3-phenylpropoxy)-1H-indene-2-carboxylic acid ethyl ester 867188-07-6P, 6-Hydroxy-1-(trans-N-methyl-N-oxoimino)-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867188-08-7P, 1-(cis-N-Methyl-N-oxoimino)-3-phenyl-6-(3-phenylpropoxy)-1H-indene-2-carboxylic acid ethyl ester 867188-09-8P, 3-(cis-N-Methyl-N-oxoimino)-1-phenyl-3H-inden-5-ol 867188-10-1P, 1-(trans-N-Methyl-N-oxoimino)-3-phenyl-6-[(5-phenylpentyl)oxy]-1H-indene-2-carboxylic acid ethyl ester 867188-11-2P, 1-(cis-N-Methyl-N-oxoimino)-3-phenyl-6-[(5-phenylpentyl)oxy]-1H-indene-2-carboxylic acid ethyl ester 867188-12-3P, 6-[2-(4-Chlorophenoxy)acetoxy]-1-(trans-N-methyl-N-oxoimino)-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867188-13-4P, 6-[2-(4-Chlorophenoxy)ethoxy]-1-(trans-N-methyl-N-oxoimino)-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867188-14-5P, 1-(trans-N-Methyl-N-oxoimino)-6-[(naphthalen-2-yl)methoxy]-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867188-15-6P, Methyl[3-phenyl-6-(3-phenylpropoxy)inden-1-ylidene]amine N-oxide 867188-16-7P, 1-(trans-N-Methyl-N-oxoimino)-6-[2-(5-methyl-2-phenylthiazol-4-yl)ethoxy]-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867188-17-8P, 6-[2-(4-Hydroxyphenyl)ethoxy]-1-(trans-N-methyl-N-oxoimino)-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867188-18-9P, 6-[2-(Adamant-1-yl)ethoxy]-1-(trans-N-methyl-N-oxoimino)-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867188-19-0P, 6-(2-Cyclohexylethoxy)-1-(trans-N-methyl-N-oxoimino)-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867188-20-3P, 1-(trans-N-Methyl-N-oxoimino)-3-phenyl-6-(3-phenyl-2-propenoxy)-1H-indene-2-carboxylic acid ethyl ester 867188-21-4P, 6-[2-(2-Fluorophenyl)ethoxy]-1-(trans-N-methyl-N-oxoimino)-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867188-22-5P, 6-[2-(3-Fluorophenyl)ethoxy]-1-(trans-N-methyl-N-oxoimino)-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867188-24-7P, 6-[2-(4-Fluorophenyl)ethoxy]-1-(trans-N-methyl-N-oxoimino)-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867188-26-9P, 1-(trans-N-Methyl-N-oxoimino)-3-phenyl-6-[2-(3-trifluoromethylphenyl)ethoxy]-1H-indene-2-carboxylic acid ethyl ester 867188-27-0P, 6-[(4-Methoxycarbonylbenzyl)oxy]-1-(trans-N-methyl-N-oxoimino)-3-phenyl-1H-

indene-2-carboxylic acid ethyl ester 867188-28-1P, 1-(trans-N-Methyl-N-oxoimino)-3-phenyl-6-(3-phenylpropoxy)-1H-indene-2-carboxylic acid ethylamide 867188-29-2P, 6-[2-[Cyclohexyl(methyl)amino]ethoxy]-1-(trans-N-methyl-N-oxoimino)-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867188-30-5P, 3-(2-Fluorophenyl)-6-methoxy-1-(trans-N-methyl-N-oxoimino)-1H-indene-2-carboxylic acid ethyl ester 867188-31-6P, 1-(trans-N-Methyl-N-oxoimino)-6-[2-(4-methylpiperazin-1-yl)ethoxy]-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867188-32-7P, (2,3-Diphenylinden-1-ylidene)methylamine N-oxide 867188-33-8P, 1-(trans-N-Methyl-N-oxoimino)-3-phenyl-6-(3-phenylpropoxy)-1H-indene-2-carboxylic acid isopropylamide 867188-34-9P, [1-(trans-N-Methyl-N-oxoimino)-3-phenyl-6-(3-phenylpropoxy)-1H-inden-2-yl]morpholin-4-ylmethanone 867188-35-0P, 1-(trans-N-Methyl-N-oxoimino)-6-[2-(morpholin-4-yl)ethoxy]-3-phenyl-1H-indene-2-carboxylic acid cyclohexylamide 867188-36-1P, 1-(trans-N-Methyl-N-oxoimino)-3-phenyl-5-(3-phenylpropoxy)-1H-indene-2-carboxylic acid ethyl ester 867188-37-2P, 1-(trans-N-Methyl-N-oxoimino)-6-(phenethyloxymethyl)-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867188-38-3P, (6-Methoxy-3-phenylinden-1-ylidene)methylamine N-oxide 867188-39-4P, 6-(2-Bromoethoxy)-1-(trans-N-methyl-N-oxoimino)-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867188-40-7P, 1-(trans-N-Methyl-N-oxoimino)-6-[2-(morpholin-4-yl)ethoxy]-3-phenyl-1H-indene-2-carboxylic acid tert-butyl ester 867188-41-8P, 4-[[[2-(Isopropylcarbamoyl)-3-(trans-N-methyl-N-oxoimino)-1-phenyl-3H-inden-5-yl]oxy]methyl]benzoic acid methyl ester 867188-42-9P, 1-(trans-N-Methyl-N-oxoimino)-6-[2-(morpholin-4-yl)ethoxy]-3-phenyl-1H-indene-2-carboxylic acid cyclopropylamide 867188-44-1P, 3-(3-Fluorophenyl)-1-(trans-N-methyl-N-oxoimino)-6-[2-(morpholin-4-yl)ethoxy]-1H-indene-2-carboxylic acid isopropylamide 867188-46-3P, [6-Methoxy-1-(cis-N-methyl-N-oxoimino)-3-phenyl-1H-inden-2-yl]acetic acid ethyl ester 867188-47-4P, [6-Methoxy-1-(trans-N-methyl-N-oxoimino)-3-phenyl-1H-inden-2-yl]acetic acid ethyl ester 867188-48-5P, 5-[2-(5-Ethylpyridin-2-yl)ethoxy]-1-(trans-N-methyl-N-oxoimino)-3-phenyl-1H-indene-2-carboxylic acid isopropylamide 867188-49-6P, 1-(trans-N-Methyl-N-oxoimino)-6-(3-phenylpropoxy)-3-(p-tolyl)-1H-indene-2-carboxylic acid ethyl ester 867188-50-9P, 1-(trans-N-Methyl-N-oxoimino)-6-(3-phenylpropoxy)-3-(thiophen-2-yl)-1H-indene-2-carboxylic acid ethyl ester 867188-51-0P, 3-(4-Chlorophenyl)-1-(trans-N-methyl-N-oxoimino)-6-(3-phenylpropoxy)-1H-indene-2-carboxylic acid ethyl ester 867188-52-1P, 3-(5-Chlorothiophen-2-yl)-1-(trans-N-methyl-N-oxoimino)-6-(3-phenylpropoxy)-1H-indene-2-carboxylic acid ethyl ester 867188-53-2P, 1-(trans-N-Methyl-N-oxoimino)-6-(3-phenylpropoxy)-3-(m-tolyl)-1H-indene-2-carboxylic acid ethyl ester 867188-54-3P, 1-(trans-N-Methyl-N-oxoimino)-3-(4-phenoxyphenyl)-6-(3-phenylpropoxy)-1H-indene-2-carboxylic acid ethyl ester 867188-55-4P, 3-(Benzodioxol-5-yl)-1-(trans-N-methyl-N-oxoimino)-6-(3-phenylpropoxy)-1H-indene-2-carboxylic acid ethyl ester 867188-56-5P, Methyl[6-(3-phenylpropoxy)-3-(pyridin-2-yl)inden-1-ylidene]amine N-oxide 867188-57-6P, 3-(Furan-2-yl)-1-(trans-N-methyl-N-oxoimino)-6-(3-phenylpropoxy)-1H-indene-2-carboxylic acid ethyl ester 867188-58-7P, 3-Ethyl-1-(trans-N-methyl-N-oxoimino)-6-(3-phenylpropoxy)-1H-indene-2-carboxylic acid ethyl ester 867188-59-8P, 3-Methyl-1-(trans-N-methyl-N-oxoimino)-6-(3-phenylpropoxy)-1H-indene-2-carboxylic acid ethyl ester 867188-60-1P, 1-(trans-N-Methyl-N-oxoimino)-6-(3-phenylpropoxy)-3-(thiophen-3-yl)-1H-indene-2-carboxylic acid ethyl ester 867188-61-2P, 3-Cyclopropyl-1-(trans-N-methyl-N-oxoimino)-6-(3-phenylpropoxy)-1H-indene-2-carboxylic acid ethyl ester 867188-62-3P, 1-(trans-N-Methyl-N-oxoimino)-6-[2-(morpholin-4-yl)ethoxy]-3-(thiophen-3-yl)-1H-indene-2-carboxylic acid ethyl ester 867188-63-4P, 3-(Benzo[b]thiophen-3-yl)-1-

(trans-N-methyl-N-oxoimino)-6-(3-phenylpropoxy)-1H-indene-2-carboxylic acid ethyl ester 867188-64-5P, 3-(1H-Imidazol-4-yl)-1-(trans-N-methyl-N-oxoimino)-6-(3-phenylpropoxy)-1H-indene-2-carboxylic acid ethyl ester 867188-65-6P, 3-(1-Ethylpropyl)-1-(trans-N-methyl-N-oxoimino)-6-(3-phenylpropoxy)-1H-indene-2-carboxylic acid ethyl ester 867188-66-7P, 1-(trans-N-Methyl-N-oxoimino)-3-phenyl-6-(3-phenylpropoxy)-1H-indene-2-carboxamide 867188-67-8P, 6-(4-Benzylmorpholin-2-ylmethoxy)-1-(trans-N-methyl-N-oxoimino)-3-phenyl-1H-indene-2-carboxylic acid isopropylamide 867188-68-9P, 1-(trans-N-Methyl-N-oxoimino)-5,6-methylenedioxy-3-phenyl-1H-indene-2-carboxylic acid isopropylamide 867188-69-0P, 1-(trans-N-Methyl-N-oxoimino)-3-phenyl-6-[2-(pyridin-2-yl)ethoxy]-1H-indene-2-carboxylic acid ethyl ester 867188-70-3P, 6-[2-(5-Ethylpyridin-2-yl)ethoxy]-1-(trans-N-methyl-N-oxoimino)-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867188-71-4P, 1-(trans-N-Methyl-N-oxoimino)-3-phenyl-6-[2-(pyridin-2-yl)ethoxy]-1H-indene-2-carboxylic acid isopropylamide 867188-72-5P, 6-[2-(5-Ethylpyridin-2-yl)ethoxy]-1-(trans-N-methyl-N-oxoimino)-3-phenyl-1H-indene-2-carboxylic acid isopropylamide 867188-73-6P, Methyl[6-[2-(morpholin-4-yl)ethoxy]-3-phenylinden-1-ylidene]amine N-oxide 867188-74-7P, 5,6-Bis(methylsulfonyloxy)-1-(trans-N-methyl-N-oxoimino)-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867188-75-8P, 1-(trans-N-Methyl-N-oxoimino)-6-[2-(morpholin-4-yl)ethoxy]-3-phenyl-1H-indene-2-carboxylic acid isobutyl ester 867188-76-9P, 1-(trans-N-Methyl-N-oxoimino)-6-[2-(morpholin-4-yl)ethoxy]-3-phenyl-1H-indene-2-carboxylic acid methyl ester 867188-77-0P, 1-(cis-N-Methyl-N-oxoimino)-6-[2-(morpholin-4-yl)ethoxy]-3-phenyl-1H-indene-2-carboxylic acid methyl ester 867188-78-1P, 1-(trans-N-Methyl-N-oxoimino)-6-[2-(morpholin-4-yl)ethoxy]-3-phenyl-1H-indene-2-carboxylic acid propyl ester 867188-79-2P, 3-(4-Fluorophenyl)-1-(trans-N-methyl-N-oxoimino)-6-[2-(morpholin-4-yl)ethoxy]-1H-indene-2-carboxylic acid ethyl ester 867188-80-5P, 1-(trans-N-Methyl-N-oxoimino)-3-phenyl-6-[(pyridin-2-yl)methoxy]-1H-indene-2-carboxylic acid ethyl ester 867188-81-6P, 1-(trans-N-Methyl-N-oxoimino)-3-phenyl-6-[(pyridin-2-yl)oxy]-1H-indene-2-carboxylic acid ethyl ester 867188-82-7P, 6-[(3-Methoxybenzyl)oxy]-1-(trans-N-methyl-N-oxoimino)-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867188-83-8P, 1-(trans-N-Methyl-N-oxoimino)-6-[2-(morpholin-4-yl)ethoxy]-3-(thiophen-3-yl)-1H-indene-2-carboxylic acid isopropylamide 867188-84-9P, 3-(1-Ethylpropyl)-1-(trans-N-methyl-N-oxoimino)-6-[2-(morpholin-4-yl)ethoxy]-1H-indene-2-carboxylic acid ethyl ester 867188-85-0P, 3-(Benzo[b]thiophen-3-yl)-1-(trans-N-methyl-N-oxoimino)-6-[2-(morpholin-4-yl)ethoxy]-1H-indene-2-carboxylic acid isopropylamide 867188-86-1P , 3-(4-Fluorophenyl)-1-(trans-N-methyl-N-oxoimino)-6-[2-(morpholin-4-yl)ethoxy]-1H-indene-2-carboxylic acid isopropylamide 867188-87-2P, 3-(1-Ethylpropyl)-1-(trans-N-methyl-N-oxoimino)-6-[2-(morpholin-4-yl)ethoxy]-1H-indene-2-carboxylic acid isopropylamide 867188-88-3P , 1-(trans-N-Methyl-N-oxoimino)-6-[2-(morpholin-4-yl)ethoxy]-3-(2,4,6-trimethylphenyl)-1H-indene-2-carboxylic acid ethyl ester 867188-89-4P, 3-(2,6-Dimethylphenyl)-1-(trans-N-methyl-N-oxoimino)-6-[2-(morpholin-4-yl)ethoxy]-1H-indene-2-carboxylic acid ethyl ester 867188-90-7P, 1-(trans-N-Methyl-N-oxoimino)-5-[2-(morpholin-4-yl)ethoxy]-3-phenyl-1H-indene-2-carboxylic acid isopropylamide 867188-91-8P, 1-(cis-N-Methyl-N-oxoimino)-6-[2-(morpholin-4-yl)ethoxy]-3-phenyl-1H-indene-2-carboxylic acid isopropyl ester 867188-92-9P, 3-(3-Fluorophenyl)-1-(trans-N-methyl-N-oxoimino)-6-[2-(pyridin-2-yl)ethoxy]-1H-indene-2-carboxylic acid isopropylamide 867188-93-0P, 6-[2-(5-Ethylpyridin-2-yl)ethoxy]-3-(3-fluorophenyl)-1-(trans-N-methyl-N-oxoimino)-1H-indene-2-carboxylic acid isopropylamide 867188-94-1P, 3-(4-Cyanophenyl)-6-[2-(morpholin-4-yl)ethoxy]-1-

(trans-N-methyl-N-oxoimino)-1H-indene-2-carboxylic acid ethyl ester 867188-95-2P, 1-(trans-N-Methyl-N-oxoimino)-3-phenyl-6-[2-(pyridin-2-yl)ethoxy]-1H-indene-2-carboxylic acid isopropyl ester
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of 1H-inden-1-imine N-oxides as selective modulators of peroxisome proliferator activated receptors)

IT 9004-10-8, Insulin, biological studies
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(hyperinsulinemia; preparation of 1H-inden-1-imine N-oxides as selective modulators of peroxisome proliferator activated receptors)

IT 94-02-0, Ethyl benzoylacetate 100-39-0, Benzyl bromide 100-52-7, Benzaldehyde, reactions 103-74-2, 2-(2-Pyridyl)ethanol 105-58-8, Diethyl carbonate 110-91-8, Morpholine, reactions 121-71-1, 3'-Hydroxyacetophenone 122-97-4, 3-Phenyl-1-propanol 495-76-1, Piperonyl alcohol 585-74-0 620-24-6, 3-Hydroxybenzyl alcohol 622-40-2, 4-(2-Hydroxyethyl)morpholine 637-59-2, 1-Bromo-3-phenylpropane 867187-77-7, 3-Phenyl-1-[3-(3-phenylpropoxy)phenyl]prop-2-enone
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of 1H-inden-1-imine N-oxides as selective modulators of peroxisome proliferator activated receptors)

IT 20850-43-5P, 5-(Chloromethyl)benzodioxole 33166-79-9P, 3-Oxo-3-(m-tolyl)propionic acid ethyl ester 34068-01-4P, 1-(3-Benzyloxyphenyl)ethanone 60760-06-7P, 3-Hydroxybenzyl chloride 62874-59-3P, 3'-(3-Phenylpropyloxy)acetophenone 73083-19-9P, 3-(3-Benzyloxyphenyl)-3-oxopropanoic acid ethyl ester 867187-56-2P, 2-(3-Hydroxybenzyl)-3-oxo-3-phenylpropionic acid ethyl ester 867187-57-3P, 6-Hydroxy-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867187-58-4P, 6-Hydroxy-1-oxo-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867187-59-5P, 1-Oxo-3-phenyl-6-(3-phenylpropoxy)-1H-indene-2-carboxylic acid ethyl ester 867187-60-8P, 1-Hydroxyimino-3-phenyl-6-(3-phenylpropyloxy)-1H-indene-2-carboxylic acid ethyl ester 867187-62-0P, 3-Phenyl-6-[2-(morpholin-4-yl)ethoxy]-1-oxo-1H-indene-2-carboxylic acid ethyl ester 867187-64-2P, 2-[(Benzodioxol-5-yl)methyl]-3-oxo-3-phenylpropionic acid ethyl ester 867187-65-3P, 5,6-Methylenedioxy-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867187-66-4P, 5,6-Methylenedioxy-1-oxo-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867187-68-6P, 3-(3-Benzyloxyphenyl)-N-isopropyl-3-oxopropionamide 867187-69-7P, 2-(3-Benzyloxybenzoyl)-N-isopropyl-3-phenylacrylamide 867187-70-0P, 5-Hydroxy-3-oxo-1-phenylindane-2-carboxylic acid isopropylamide 867187-71-1P, 6-Hydroxy-1-oxo-3-phenyl-1H-indene-2-carboxylic acid isopropylamide 867187-72-2P, 6-[2-(Morpholin-4-yl)ethoxy]-1-oxo-3-phenyl-1H-indene-2-carboxylic acid isopropylamide 867187-73-3P, 3'-(3-Phenylpropyloxy)benzoylacetic acid ethyl ester 867187-74-4P, 2-Benzoyl-3-[3'-(3-phenylpropyloxy)phenyl]-3-oxopropanoic acid ethyl ester 867187-76-6P, 3-Phenyl-6-(3-phenylpropoxy)indan-1-one 867187-78-8P, 2-Bromo-3-phenyl-6-(3-phenylpropoxy)indan-1-one 867187-79-9P, 1-Oxo-3-phenyl-6-(3-phenylpropoxy)-1H-indene-2-carbonitrile 867187-80-2P, trans-1-Hydroxyimino-3-phenyl-6-[(3-phenylpropyl)oxy]-1H-indene-2-carbonitrile 867187-84-6P, 2-(3-Methylbenzoyl)-3-phenylacrylic acid ethyl ester 867187-85-7P, 5-Methyl-3-oxo-1-phenylindane-2-carboxylic acid ethyl ester 867187-86-8P, 6-Methyl-1-oxo-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867187-87-9P, 6-Bromomethyl-1-oxo-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867187-88-0P, 6-(Morpholin-4-ylmethyl)-1-oxo-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867187-90-4P, 3-Phenyl-6-(3-phenylpropyloxy)-1-oxo-1H-indene-2-carboxylic acid methyl ester 867187-91-5P,

3-Phenyl-6-(3-phenylpropyloxy)-1-oxo-1H-indene-2-carboxylic acid 867187-92-6P, 3-Phenyl-6-(3-phenylpropyloxy)-1-oxo-1H-indene-2-carboxylic acid cyclohexylamide 867187-94-8P, 2-(Isopropylcarbamoyl)-1-oxo-3-phenyl-1H-inden-5-yl acetate 867187-95-9P, 5-Hydroxy-1-(trans-N-methyl-N-oxoimino)-3-phenyl-1H-indene-2-carboxylic acid isopropylamide
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 1H-inden-1-imine N-oxides as selective modulators of peroxisome proliferator activated receptors)

IT 867187-81-3P, cis-1-Hydroxyimino-3-phenyl-6-[(3-phenylpropyl)oxy]-1H-indene-2-carbonitrile 867187-82-4P, 1-(trans-Methoxyimino)-3-phenyl-6-(3-phenylpropoxy)-1H-indene-2-carbonitrile
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of 1H-inden-1-imine N-oxides as selective modulators of peroxisome proliferator activated receptors)

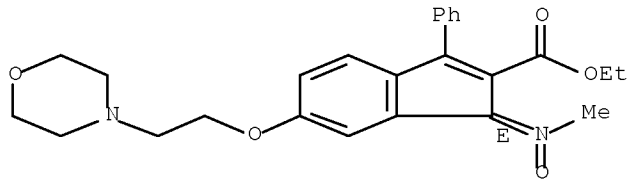
IT 50-99-7, Glucose, biological studies
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(reducers of blood glucose levels; preparation of 1H-inden-1-imine N-oxides as selective modulators of peroxisome proliferator activated receptors)

IT 867187-61-9P, 1-(trans-N-Methyl-N-oxoimino)-6-[2-(morpholin-4-yl)ethoxy]-3-phenyl-1H-indene-2-carboxylic acid ethyl ester
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(drug candidate; preparation of 1H-inden-1-imine N-oxides as selective modulators of peroxisome proliferator activated receptors)

RN 867187-61-9 ZCAPLUS

CN 1H-Indene-2-carboxylic acid, 1-(methyloxidoimino)-6-[2-(4-morpholinyl)ethoxy]-3-phenyl-, ethyl ester, (1E)- (CA INDEX NAME)

Double bond geometry as shown.



IT 867187-55-1P, 1-(trans-N-Methyl-N-oxoimino)-3-phenyl-6-(3-phenylpropoxy)-1H-indene-2-carboxylic acid ethyl ester 867187-67-5P, 1-(trans-N-Methyl-N-oxoimino)-6-[2-(morpholin-4-yl)ethoxy]-3-phenyl-1H-indene-2-carboxylic acid isopropylamide 867187-75-5P, 1-(trans-N-Methyl-N-oxoimino)-3-phenyl-6-(3-phenylpropoxy)-1H-indene-2-carbonitrile 867187-83-5P, 1-(trans-N-Methyl-N-oxoimino)-6-[(morpholin-4-yl)methyl]-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867187-89-1P, 1-(trans-N-Methyl-N-oxoimino)-3-phenyl-6-(3-phenylpropoxy)-1H-indene-2-carboxylic acid cyclohexylamide 867187-93-7P, 1-(trans-N-Methyl-N-oxoimino)-3-phenyl-5-[2-(pyridin-2-yl)ethoxy]-1H-indene-2-carboxylic acid isopropylamide 867187-96-0P, 1-(cis-N-Methyl-N-oxoimino)-6-[2-(morpholin-4-yl)ethoxy]-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867187-98-2P, 6-Methoxy-1-(trans-N-methyl-N-oxoimino)-3-phenyl-1H-indene-2-carboxylic

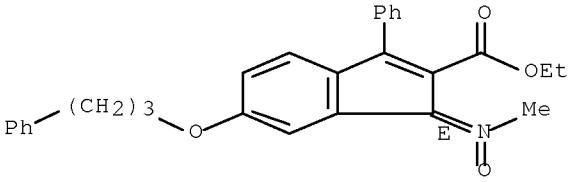
acid ethyl ester 867187-99-3P, 1-(trans-N-Isopropyl-N-oxoimino)-6-methoxy-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867188-00-9P, 1-(trans-N-Benzyl-N-oxoimino)-6-methoxy-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867188-01-0P, 1-(trans-N-Ethyl-N-oxoimino)-6-methoxy-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867188-02-1P, 6-Methoxy-1-[trans-N-(3-phenylpropyl)-N-oxoimino]-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867188-03-2P, 6-Methoxy-1-[trans-N-(3-methyl-2-butenyl)-N-oxoimino]-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867188-04-3P, 1-(trans-N-Isobutyl-N-oxoimino)-6-methoxy-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867188-05-4P, 1-(trans-N-Methyl-N-oxoimino)-6-phenethyloxy-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867188-08-7P, 1-(cis-N-Methyl-N-oxoimino)-3-phenyl-6-(3-phenylpropoxy)-1H-indene-2-carboxylic acid ethyl ester 867188-10-1P, 1-(trans-N-Methyl-N-oxoimino)-3-phenyl-6-[(5-phenylpentyl)oxy]-1H-indene-2-carboxylic acid ethyl ester 867188-11-2P, 1-(cis-N-Methyl-N-oxoimino)-3-phenyl-6-[(5-phenylpentyl)oxy]-1H-indene-2-carboxylic acid ethyl ester 867188-12-3P, 6-[2-(4-Chlorophenoxy)acetoxy]-1-(trans-N-methyl-N-oxoimino)-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867188-13-4P, 6-[2-(4-Chlorophenoxy)ethoxy]-1-(trans-N-methyl-N-oxoimino)-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867188-14-5P, 1-(trans-N-Methyl-N-oxoimino)-6-[(naphthalen-2-yl)methoxy]-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867188-16-7P, 1-(trans-N-Methyl-N-oxoimino)-6-[2-(5-methyl-2-phenylthiazol-4-yl)ethoxy]-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867188-17-8P, 6-[2-(4-Hydroxyphenyl)ethoxy]-1-(trans-N-methyl-N-oxoimino)-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867188-18-9P, 6-[2-(Adamant-1-yl)ethoxy]-1-(trans-N-methyl-N-oxoimino)-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867188-19-0P, 6-(2-Cyclohexylethoxy)-1-(trans-N-methyl-N-oxoimino)-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867188-20-3P, 1-(trans-N-Methyl-N-oxoimino)-3-phenyl-6-(3-phenyl-2-propenoxy)-1H-indene-2-carboxylic acid ethyl ester 867188-21-4P, 6-[2-(2-Fluorophenyl)ethoxy]-1-(trans-N-methyl-N-oxoimino)-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867188-22-5P, 6-[2-(3-Fluorophenyl)ethoxy]-1-(trans-N-methyl-N-oxoimino)-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867188-24-7P, 6-[2-(4-Fluorophenyl)ethoxy]-1-(trans-N-methyl-N-oxoimino)-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867188-26-9P, 1-(trans-N-Methyl-N-oxoimino)-3-phenyl-6-[2-(3-trifluoromethylphenyl)ethoxy]-1H-indene-2-carboxylic acid ethyl ester 867188-27-0P, 6-[(4-Methoxycarbonylbenzyl)oxy]-1-(trans-N-methyl-N-oxoimino)-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867188-28-1P, 1-(trans-N-Methyl-N-oxoimino)-3-phenyl-6-(3-phenylpropoxy)-1H-indene-2-carboxylic acid ethylamide 867188-29-2P, 6-[2-[Cyclohexyl(methyl)amino]ethoxy]-1-(trans-N-methyl-N-oxoimino)-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867188-30-5P, 3-(2-Fluorophenyl)-6-methoxy-1-(trans-N-methyl-N-oxoimino)-1H-indene-2-carboxylic acid ethyl ester 867188-31-6P, 1-(trans-N-Methyl-N-oxoimino)-6-[2-(4-methylpiperazin-1-yl)ethoxy]-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867188-33-8P, 1-(trans-N-Methyl-N-oxoimino)-3-phenyl-6-(3-phenylpropoxy)-1H-indene-2-carboxylic acid isopropylamide 867188-35-0P, 1-(trans-N-Methyl-N-oxoimino)-6-[2-(morpholin-4-yl)ethoxy]-3-phenyl-1H-indene-2-carboxylic acid cyclohexylamide 867188-36-1P, 1-(trans-N-Methyl-N-oxoimino)-3-phenyl-5-(3-phenylpropoxy)-1H-indene-2-carboxylic acid ethyl ester 867188-39-4P, 6-(2-Bromoethoxy)-1-(trans-N-methyl-N-oxoimino)-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867188-40-7P, 1-(trans-N-Methyl-N-oxoimino)-6-[2-(morpholin-4-yl)ethoxy]-3-phenyl-1H-

indene-2-carboxylic acid tert-butyl ester 867188-41-8P, 4-[[[2-(Isopropylcarbamoyl)-3-(trans-N-methyl-N-oxoimino)-1-phenyl-3H-inden-5-yl]oxy]methyl]benzoic acid methyl ester 867188-42-9P, 1-(trans-N-Methyl-N-oxoimino)-6-[2-(morpholin-4-yl)ethoxy]-3-phenyl-1H-indene-2-carboxylic acid cyclopropylamide 867188-44-1P, 3-(3-Fluorophenyl)-1-(trans-N-methyl-N-oxoimino)-6-[2-(morpholin-4-yl)ethoxy]-1H-indene-2-carboxylic acid isopropylamide 867188-48-5P, 5-[2-(5-Ethylpyridin-2-yl)ethoxy]-1-(trans-N-methyl-N-oxoimino)-3-phenyl-1H-indene-2-carboxylic acid isopropylamide 867188-49-6P, 1-(trans-N-Methyl-N-oxoimino)-6-(3-phenylpropoxy)-3-(p-tolyl)-1H-indene-2-carboxylic acid ethyl ester 867188-51-0P, 3-(4-Chlorophenyl)-1-(trans-N-methyl-N-oxoimino)-6-(3-phenylpropoxy)-1H-indene-2-carboxylic acid ethyl ester 867188-53-2P, 1-(trans-N-Methyl-N-oxoimino)-6-(3-phenylpropoxy)-3-(m-tolyl)-1H-indene-2-carboxylic acid ethyl ester 867188-54-3P, 1-(trans-N-Methyl-N-oxoimino)-3-(4-phenoxyphenyl)-6-(3-phenylpropoxy)-1H-indene-2-carboxylic acid ethyl ester 867188-55-4P, 3-(Benzodioxol-5-yl)-1-(trans-N-methyl-N-oxoimino)-6-(3-phenylpropoxy)-1H-indene-2-carboxylic acid ethyl ester 867188-66-7P, 1-(trans-N-Methyl-N-oxoimino)-3-phenyl-6-(3-phenylpropoxy)-1H-indene-2-carboxamide 867188-67-8P, 6-(4-Benzylmorpholin-2-ylmethoxy)-1-(trans-N-methyl-N-oxoimino)-3-phenyl-1H-indene-2-carboxylic acid isopropylamide 867188-69-0P, 1-(trans-N-Methyl-N-oxoimino)-3-phenyl-6-[2-(pyridin-2-yl)ethoxy]-1H-indene-2-carboxylic acid ethyl ester 867188-70-3P, 6-[2-(5-Ethylpyridin-2-yl)ethoxy]-1-(trans-N-methyl-N-oxoimino)-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867188-71-4P, 1-(trans-N-Methyl-N-oxoimino)-3-phenyl-6-[2-(pyridin-2-yl)ethoxy]-1H-indene-2-carboxylic acid isopropylamide 867188-72-5P, 6-[2-(5-Ethylpyridin-2-yl)ethoxy]-1-(trans-N-methyl-N-oxoimino)-3-phenyl-1H-indene-2-carboxylic acid isopropylamide 867188-75-8P, 1-(trans-N-Methyl-N-oxoimino)-6-[2-(morpholin-4-yl)ethoxy]-3-phenyl-1H-indene-2-carboxylic acid isobutyl ester 867188-76-9P, 1-(trans-N-Methyl-N-oxoimino)-6-[2-(morpholin-4-yl)ethoxy]-3-phenyl-1H-indene-2-carboxylic acid methyl ester 867188-77-0P, 1-(cis-N-Methyl-N-oxoimino)-6-[2-(morpholin-4-yl)ethoxy]-3-phenyl-1H-indene-2-carboxylic acid methyl ester 867188-78-1P, 1-(trans-N-Methyl-N-oxoimino)-6-[2-(morpholin-4-yl)ethoxy]-3-phenyl-1H-indene-2-carboxylic acid propyl ester 867188-79-2P, 3-(4-Fluorophenyl)-1-(trans-N-methyl-N-oxoimino)-6-[2-(morpholin-4-yl)ethoxy]-1H-indene-2-carboxylic acid ethyl ester 867188-80-5P, 1-(trans-N-Methyl-N-oxoimino)-3-phenyl-6-[(pyridin-2-yl)methoxy]-1H-indene-2-carboxylic acid ethyl ester 867188-82-7P, 6-[(3-Methoxybenzyl)oxy]-1-(trans-N-methyl-N-oxoimino)-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867188-86-1P, 3-(4-Fluorophenyl)-1-(trans-N-methyl-N-oxoimino)-6-[2-(morpholin-4-yl)ethoxy]-1H-indene-2-carboxylic acid isopropylamide 867188-88-3P, 1-(trans-N-Methyl-N-oxoimino)-6-[2-(morpholin-4-yl)ethoxy]-3-(2,4,6-trimethylphenyl)-1H-indene-2-carboxylic acid ethyl ester 867188-89-4P, 3-(2,6-Dimethylphenyl)-1-(trans-N-methyl-N-oxoimino)-6-[2-(morpholin-4-yl)ethoxy]-1H-indene-2-carboxylic acid ethyl ester 867188-90-7P, 1-(trans-N-Methyl-N-oxoimino)-5-[2-(morpholin-4-yl)ethoxy]-3-phenyl-1H-indene-2-carboxylic acid isopropylamide 867188-91-8P, 1-(cis-N-Methyl-N-oxoimino)-6-[2-(morpholin-4-yl)ethoxy]-3-phenyl-1H-indene-2-carboxylic acid isopropyl ester 867188-92-9P, 3-(3-Fluorophenyl)-1-(trans-N-methyl-N-oxoimino)-6-[2-(pyridin-2-yl)ethoxy]-1H-indene-2-carboxylic acid isopropylamide 867188-93-0P, 6-[2-(5-Ethylpyridin-2-yl)ethoxy]-3-(3-fluorophenyl)-1-(trans-N-methyl-N-oxoimino)-1H-indene-2-carboxylic acid isopropylamide 867188-94-1P, 3-(4-Cyanophenyl)-6-[2-(morpholin-4-yl)ethoxy]-1-(trans-N-methyl-N-oxoimino)-1H-indene-2-carboxylic acid ethyl ester

867188-95-2P, 1-(trans-N-Methyl-N-oxoimino)-3-phenyl-6-[2-(pyridin-2-yl)ethoxy]-1H-indene-2-carboxylic acid isopropyl ester
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of 1H-inden-1-imine N-oxides as selective modulators of peroxisome proliferator activated receptors)

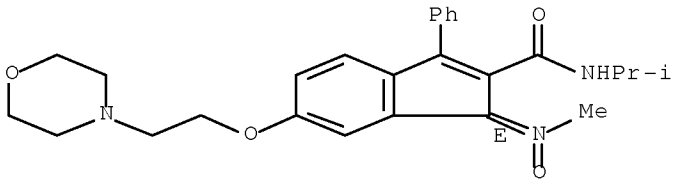
RN 867187-55-1 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-(methyloxidoimino)-3-phenyl-6-(3-phenylpropoxy)-, ethyl ester, (1E)- (CA INDEX NAME)

Double bond geometry as shown.



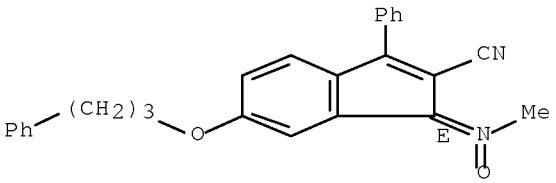
RN 867187-67-5 ZCAPLUS
CN 1H-Indene-2-carboxamide, N-(1-methylethyl)-1-(methyloxidoimino)-6-[2-(4-morpholinyl)ethoxy]-3-phenyl-, (1E)- (CA INDEX NAME)

Double bond geometry as shown.



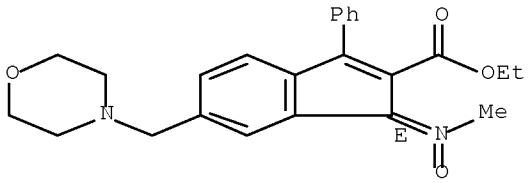
RN 867187-75-5 ZCAPLUS
CN 1H-Indene-2-carbonitrile, 1-(methyloxidoimino)-3-phenyl-6-(3-phenylpropoxy)-, (1E)- (CA INDEX NAME)

Double bond geometry as shown.



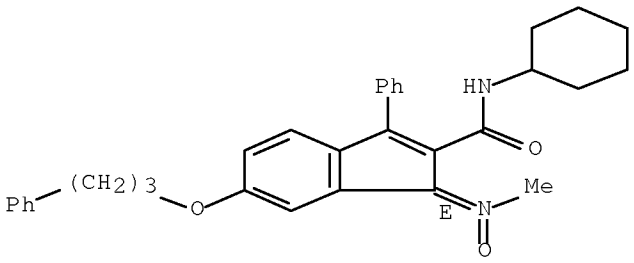
RN 867187-83-5 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-(methyloxidoimino)-6-(4-morpholinylmethyl)-3-phenyl-, ethyl ester, (1E)- (CA INDEX NAME)

Double bond geometry as shown.



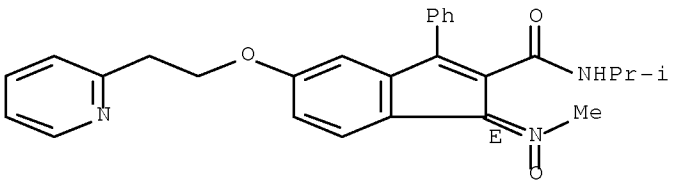
RN 867187-89-1 ZCAPLUS
CN 1H-Indene-2-carboxamide, N-cyclohexyl-1-(methyloxidoimino)-3-phenyl-6-(3-phenylpropoxy)-, (1E)- (CA INDEX NAME)

Double bond geometry as shown.



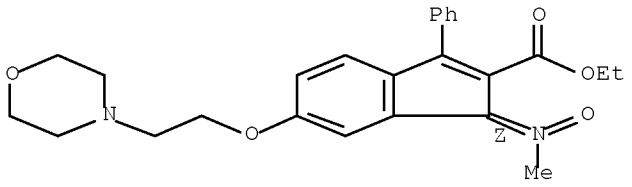
RN 867187-93-7 ZCAPLUS
CN 1H-Indene-2-carboxamide, N-(1-methylethyl)-1-(methyloxidoimino)-3-phenyl-5-[2-(2-pyridinyl)ethoxy]-, (1E)- (CA INDEX NAME)

Double bond geometry as shown.



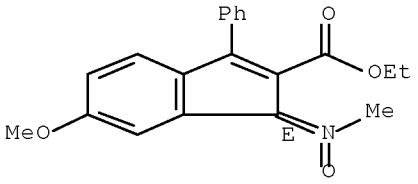
RN 867187-96-0 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-(methyloxidoimino)-6-[2-(4-morpholinyl)ethoxy]-3-phenyl-, ethyl ester, (1Z)- (CA INDEX NAME)

Double bond geometry as shown.



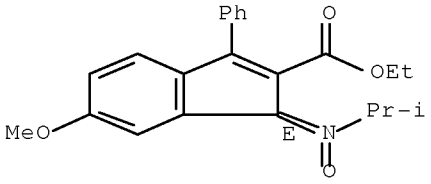
RN 867187-98-2 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 6-methoxy-1-(methyloxidoimino)-3-phenyl-, ethyl ester, (1E)- (CA INDEX NAME)

Double bond geometry as shown.



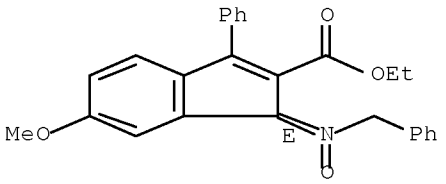
RN 867187-99-3 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 6-methoxy-1-[(1-methylethyl)oxidoimino]-3-phenyl-, ethyl ester, (1E)- (CA INDEX NAME)

Double bond geometry as shown.



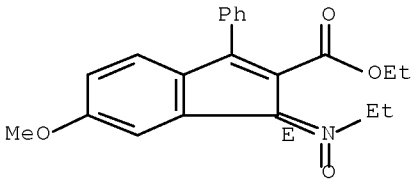
RN 867188-00-9 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 6-methoxy-1-[oxido(phenylmethyl)imino]-3-phenyl-, ethyl ester, (1E)- (CA INDEX NAME)

Double bond geometry as shown.



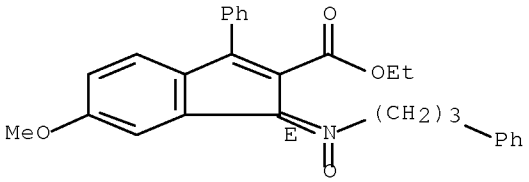
RN 867188-01-0 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-(ethyloxidoimino)-6-methoxy-3-phenyl-, ethyl ester, (1E)- (CA INDEX NAME)

Double bond geometry as shown.



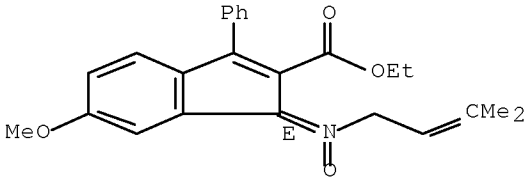
RN 867188-02-1 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 6-methoxy-1-[oxido(3-phenylpropyl)imino]-3-phenyl-, ethyl ester, (1E)- (CA INDEX NAME)

Double bond geometry as shown.



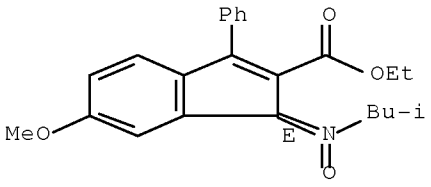
RN 867188-03-2 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 6-methoxy-1-[(3-methyl-2-buten-1-yl)oxidoimino]-3-phenyl-, ethyl ester, (1E)- (CA INDEX NAME)

Double bond geometry as shown.



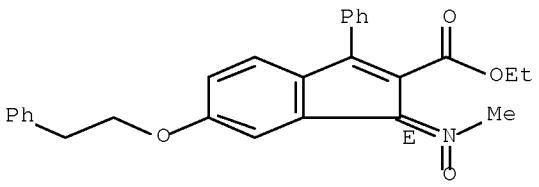
RN 867188-04-3 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 6-methoxy-1-[(2-methylpropyl)oxidoimino]-3-phenyl-, ethyl ester, (1E)- (CA INDEX NAME)

Double bond geometry as shown.



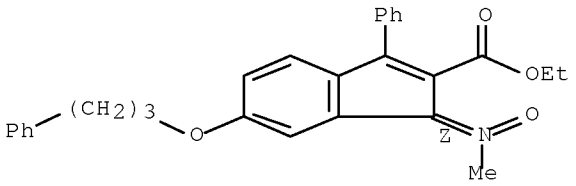
RN 867188-05-4 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-(methyloxidoimino)-3-phenyl-6-(2-phenylethoxy)-, ethyl ester, (1E)- (CA INDEX NAME)

Double bond geometry as shown.



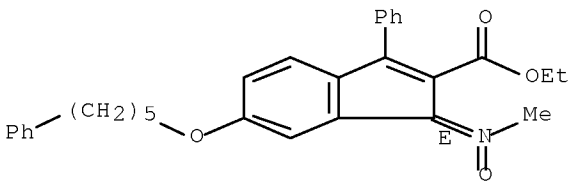
RN 867188-08-7 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-(methyloxidoimino)-3-phenyl-6-(3-phenylpropoxy)-, ethyl ester, (1Z)- (CA INDEX NAME)

Double bond geometry as shown.



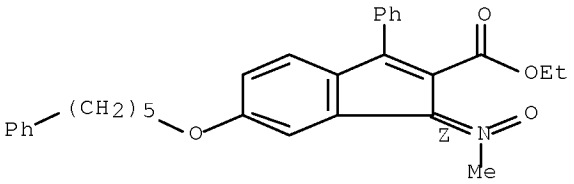
RN 867188-10-1 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-(methyloxidoimino)-3-phenyl-6-[(5-phenylpentyl)oxy]-, ethyl ester, (1E)- (CA INDEX NAME)

Double bond geometry as shown.



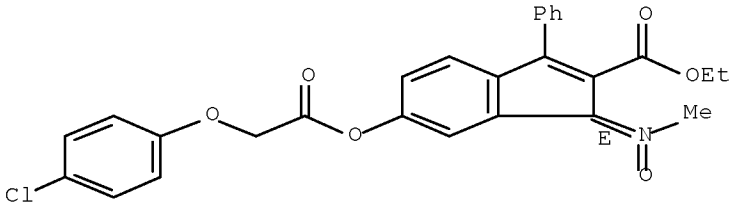
RN 867188-11-2 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-(methyloxidoimino)-3-phenyl-6-[(5-phenylpentyl)oxy]-, ethyl ester, (1Z)- (CA INDEX NAME)

Double bond geometry as shown.



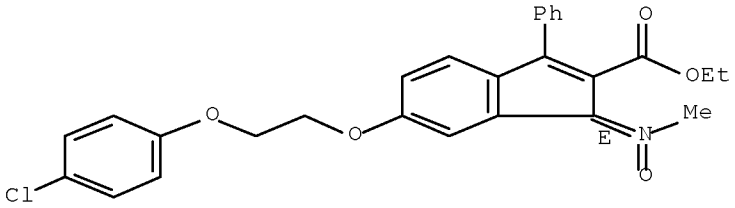
RN 867188-12-3 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 6-[[2-(4-chlorophenoxy)acetyl]oxy]-1-(methyloxidoimino)-3-phenyl-, ethyl ester, (1E)- (CA INDEX NAME)

Double bond geometry as shown.



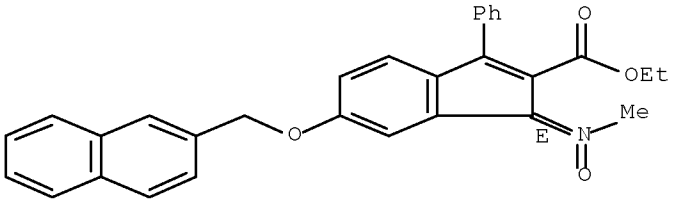
RN 867188-13-4 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 6-[2-(4-chlorophenoxy)ethoxy]-1-(methyloxidoimino)-3-phenyl-, ethyl ester, (1E)- (CA INDEX NAME)

Double bond geometry as shown.



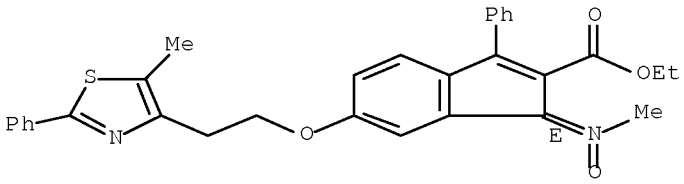
RN 867188-14-5 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-(methyloxidoimino)-6-(2-naphthalenylmethoxy)-3-phenyl-, ethyl ester, (1E)- (CA INDEX NAME)

Double bond geometry as shown.



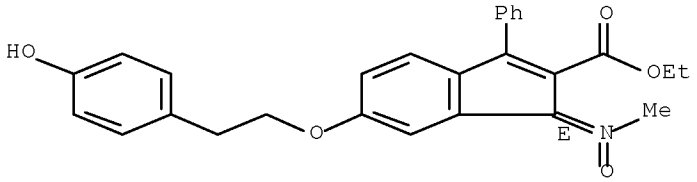
RN 867188-16-7 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-(methyloxidoimino)-6-[2-(5-methyl-2-phenyl-4-thiazolyl)ethoxy]-3-phenyl-, ethyl ester, (1E)- (CA INDEX NAME)

Double bond geometry as shown.



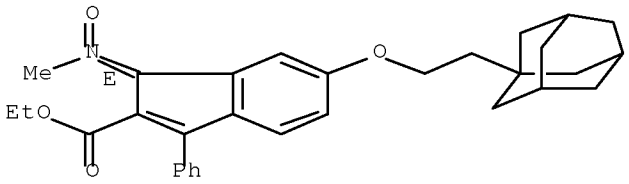
RN 867188-17-8 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 6-[2-(4-hydroxyphenyl)ethoxy]-1-(methyloxidoimino)-3-phenyl-, ethyl ester, (1E)- (CA INDEX NAME)

Double bond geometry as shown.



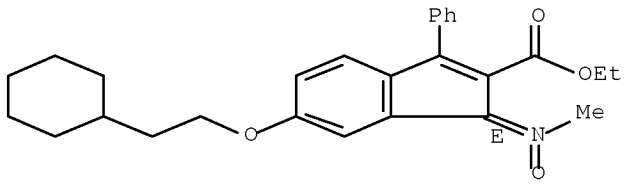
RN 867188-18-9 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-(methyloxidoimino)-3-phenyl-6-(2-tricyclo[3.3.1.13,7]dec-1-ylethoxy)-, ethyl ester, (1E)- (CA INDEX NAME)

Double bond geometry as shown.



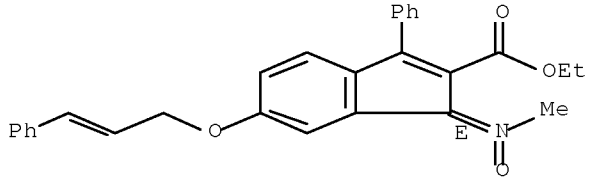
RN 867188-19-0 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 6-(2-cyclohexylethoxy)-1-(methyloxidoimino)-3-phenyl-, ethyl ester, (1E)- (CA INDEX NAME)

Double bond geometry as shown.



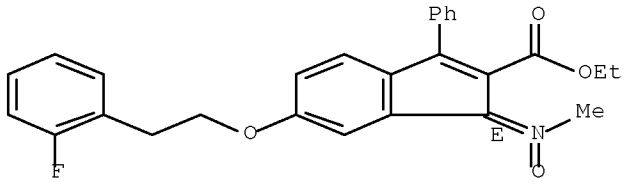
RN 867188-20-3 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-(methyloxidoimino)-3-phenyl-6-[(3-phenyl-2-propen-1-yl)oxy]-, ethyl ester, (1E)- (CA INDEX NAME)

Double bond geometry as described by E or Z.



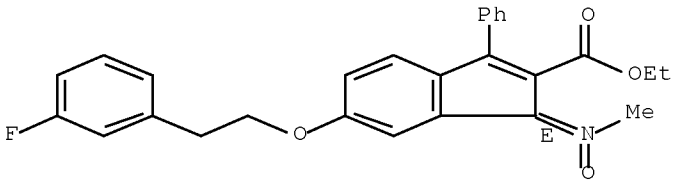
RN 867188-21-4 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 6-[2-(2-fluorophenyl)ethoxy]-1-(methyloxidoimino)-3-phenyl-, ethyl ester, (1E)- (CA INDEX NAME)

Double bond geometry as shown.



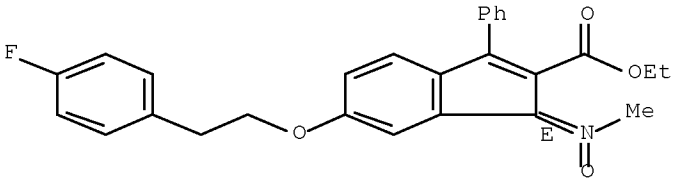
RN 867188-22-5 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 6-[2-(3-fluorophenyl)ethoxy]-1-(methyloxidoimino)-3-phenyl-, ethyl ester, (1E)- (CA INDEX NAME)

Double bond geometry as shown.



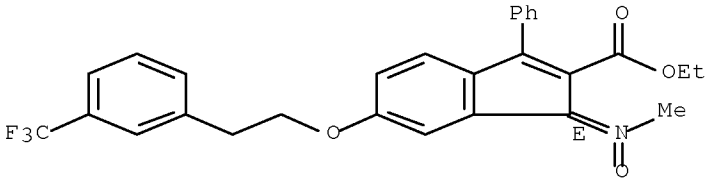
RN 867188-24-7 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 6-[2-(4-fluorophenyl)ethoxy]-1-(methyloxidoimino)-3-phenyl-, ethyl ester, (1E)- (CA INDEX NAME)

Double bond geometry as shown.



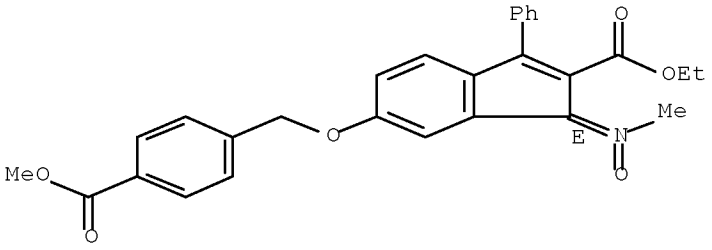
RN 867188-26-9 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-(methyloxidoimino)-3-phenyl-6-[2-[3-(trifluoromethyl)phenyl]ethoxy]-, ethyl ester, (1E)- (CA INDEX NAME)

Double bond geometry as shown.



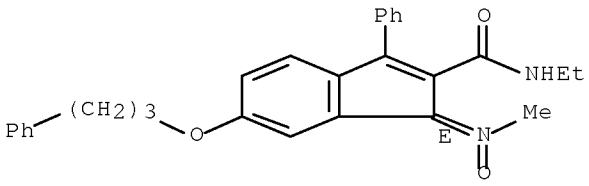
RN 867188-27-0 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 6-[[4-(methoxycarbonyl)phenyl]methoxy]-1-(methyloxidoimino)-3-phenyl-, ethyl ester, (1E)- (CA INDEX NAME)

Double bond geometry as shown.



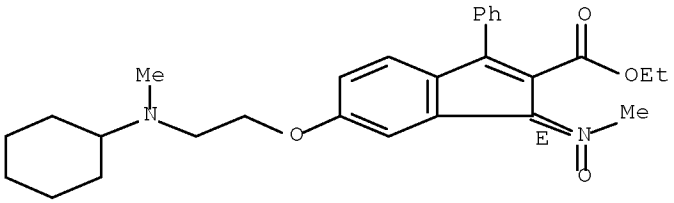
RN 867188-28-1 ZCAPLUS
CN 1H-Indene-2-carboxamide, N-ethyl-1-(methyloxidoimino)-3-phenyl-6-(3-phenylpropoxy)-, (1E)- (CA INDEX NAME)

Double bond geometry as shown.



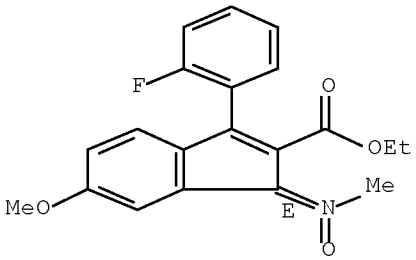
RN 867188-29-2 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 6-[2-(cyclohexylmethylamino)ethoxy]-1-(methyloxidoimino)-3-phenyl-, ethyl ester, (1E)- (CA INDEX NAME)

Double bond geometry as shown.



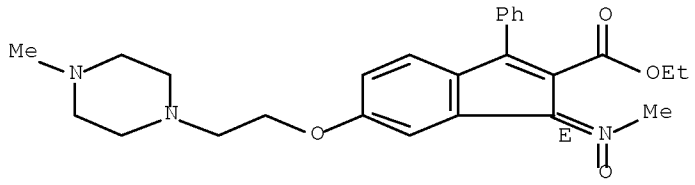
RN 867188-30-5 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 3-(2-fluorophenyl)-6-methoxy-1-(methyloxidoimino)-, ethyl ester, (1E)- (CA INDEX NAME)

Double bond geometry as shown.



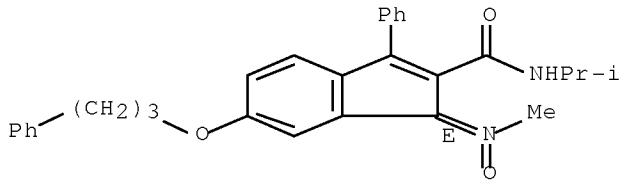
RN 867188-31-6 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-(methyloxidoimino)-6-[2-(4-methyl-1-piperazinyl)ethoxy]-3-phenyl-, ethyl ester, (1E)- (CA INDEX NAME)

Double bond geometry as shown.



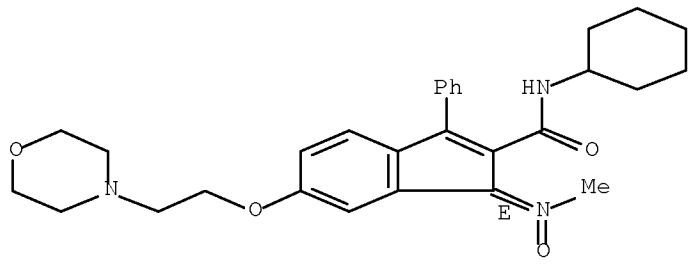
RN 867188-33-8 ZCAPLUS
CN 1H-Indene-2-carboxamide, N-(1-methylethyl)-1-(methyloxidoimino)-3-phenyl-6-(3-phenylpropoxy)-, (1E)- (CA INDEX NAME)

Double bond geometry as shown.



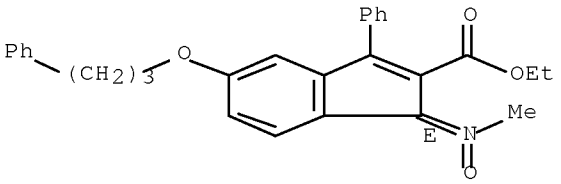
RN 867188-35-0 ZCAPLUS
CN 1H-Indene-2-carboxamide, N-cyclohexyl-1-(methyloxidoimino)-6-[2-(4-morpholinyl)ethoxy]-3-phenyl-, (1E)- (CA INDEX NAME)

Double bond geometry as shown.



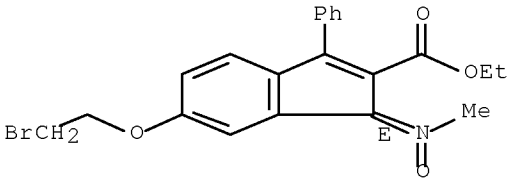
RN 867188-36-1 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-(methyloxidoimino)-3-phenyl-5-(3-phenylpropoxy)-, ethyl ester, (1E)- (CA INDEX NAME)

Double bond geometry as shown.



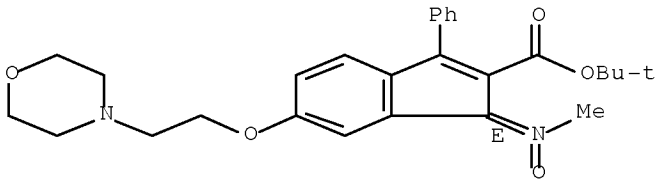
RN 867188-39-4 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 6-(2-bromoethoxy)-1-(methyloxidoimino)-3-phenyl-, ethyl ester, (1E)- (CA INDEX NAME)

Double bond geometry as shown.



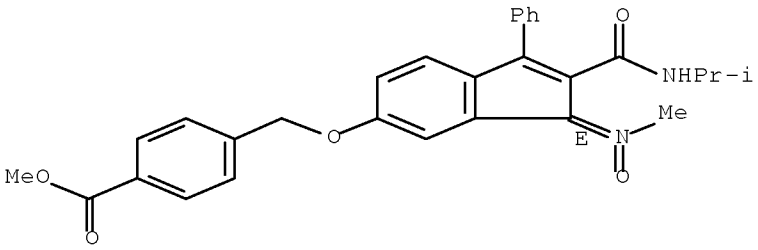
RN 867188-40-7 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-(methyloxidoimino)-6-[2-(4-morpholinyl)ethoxy]-3-phenyl-, 1,1-dimethylethyl ester, (1E)- (CA INDEX NAME)

Double bond geometry as shown.



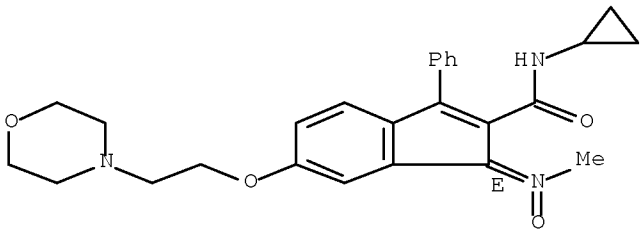
RN 867188-41-8 ZCAPLUS
CN Benzoic acid, 4-[[[(1E)-2-[[(1-methylethyl)amino]carbonyl]-1-(methyloxidoimino)-3-phenyl-1H-inden-6-yl]oxy]methyl]-, methyl ester (CA INDEX NAME)

Double bond geometry as shown.



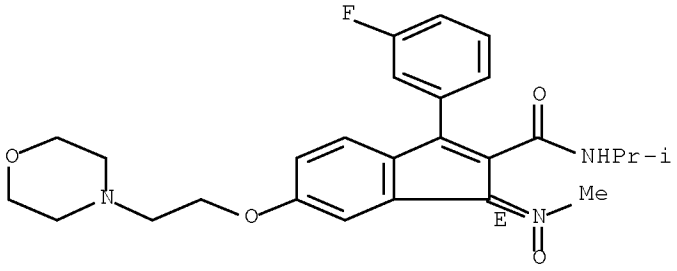
RN 867188-42-9 ZCAPLUS
CN 1H-Indene-2-carboxamide, N-cyclopropyl-1-(methyloxidoimino)-6-[2-(4-morpholinyl)ethoxy]-3-phenyl-, (1E)- (CA INDEX NAME)

Double bond geometry as shown.



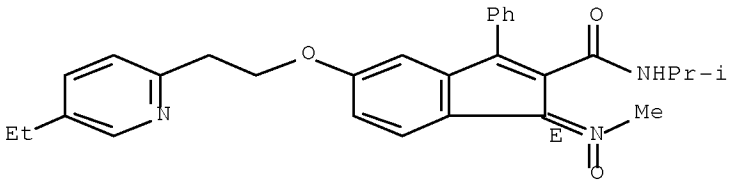
RN 867188-44-1 ZCAPLUS
CN 1H-Indene-2-carboxamide, 3-(3-fluorophenyl)-N-(1-methylethyl)-1-(methyloxidoimino)-6-[2-(4-morpholinyl)ethoxy]-, (1E)- (CA INDEX NAME)

Double bond geometry as shown.



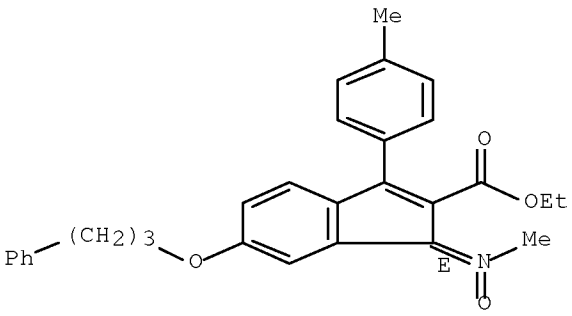
RN 867188-48-5 ZCAPLUS
CN 1H-Indene-2-carboxamide, 5-[2-(5-ethyl-2-pyridinyl)ethoxy]-N-(1-methylethyl)-1-(methyloxidoimino)-3-phenyl-, (1E)- (CA INDEX NAME)

Double bond geometry as shown.



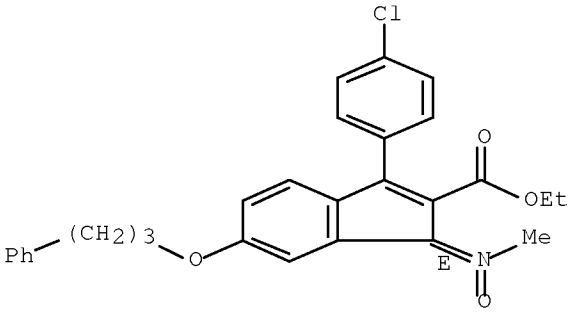
RN 867188-49-6 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-(methyloxidoimino)-3-(4-methylphenyl)-6-(3-phenylpropoxy)-, ethyl ester, (1E)- (CA INDEX NAME)

Double bond geometry as shown.



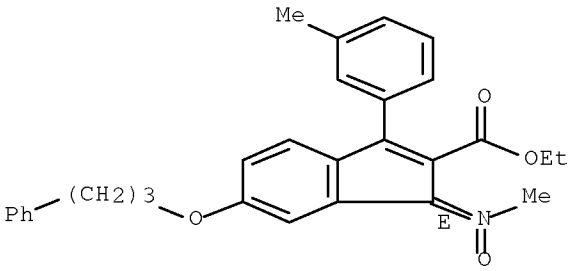
RN 867188-51-0 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 3-(4-chlorophenyl)-1-(methyloxidoimino)-6-(3-phenylpropoxy)-, ethyl ester, (1E)- (CA INDEX NAME)

Double bond geometry as shown.



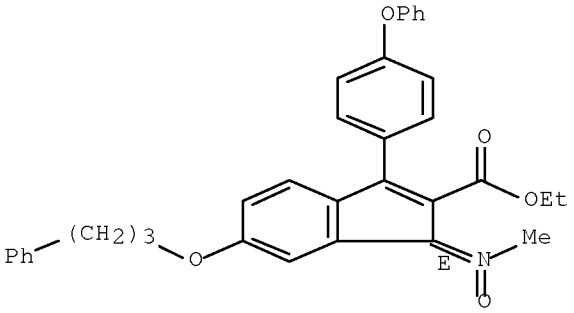
RN 867188-53-2 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-(methyloxidoimino)-3-(3-methylphenyl)-6-(3-phenylpropoxy)-, ethyl ester, (1E)- (CA INDEX NAME)

Double bond geometry as shown.



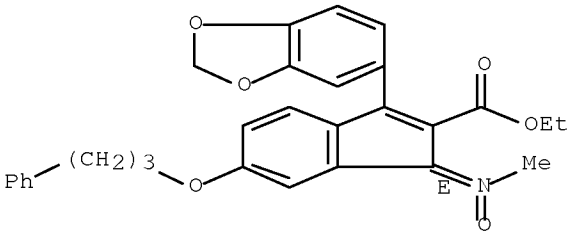
RN 867188-54-3 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-(methyloxidoimino)-3-(4-phenoxyphenyl)-6-(3-phenylpropoxy)-, ethyl ester, (1E)- (CA INDEX NAME)

Double bond geometry as shown.



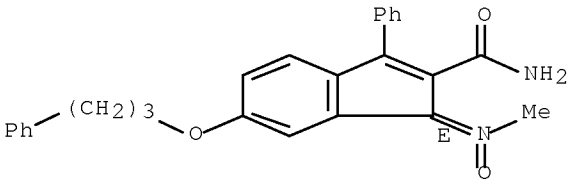
RN 867188-55-4 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 3-(1,3-benzodioxol-5-yl)-1-(methyloxidoimino)-6-(3-phenylpropoxy)-, ethyl ester, (1E)- (CA INDEX NAME)

Double bond geometry as shown.



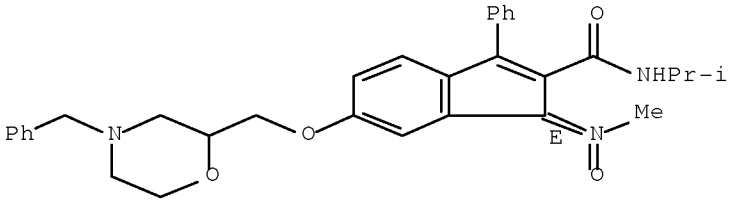
RN 867188-66-7 ZCAPLUS
CN 1H-Indene-2-carboxamide, 1-(methyloxidoimino)-3-phenyl-6-(3-phenylpropoxy)-, (1E)- (CA INDEX NAME)

Double bond geometry as shown.



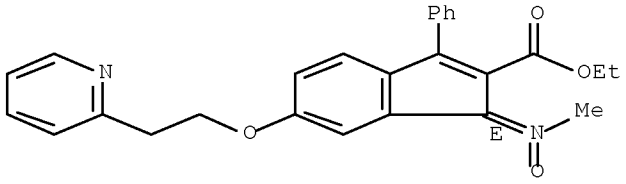
RN 867188-67-8 ZCAPLUS
CN 1H-Indene-2-carboxamide, N-(1-methylethyl)-1-(methyloxidoimino)-3-phenyl-6-[[4-(phenylmethyl)-2-morpholinyl]methoxy]-, (1E)- (CA INDEX NAME)

Double bond geometry as shown.



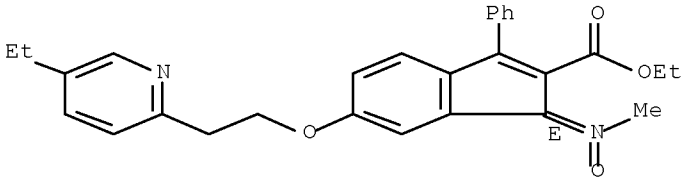
RN 867188-69-0 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-(methyloxidoimino)-3-phenyl-6-[2-(2-pyridinyl)ethoxy]-, ethyl ester, (1E)- (CA INDEX NAME)

Double bond geometry as shown.



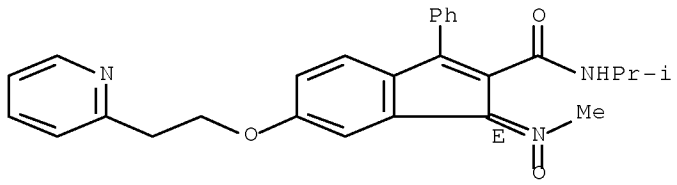
RN 867188-70-3 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 6-[2-(5-ethyl-2-pyridinyl)ethoxy]-1-(methyloxidoimino)-3-phenyl-, ethyl ester, (1E)- (CA INDEX NAME)

Double bond geometry as shown.



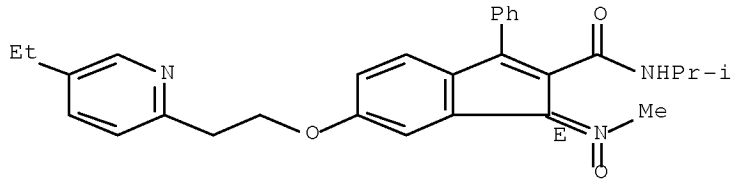
RN 867188-71-4 ZCAPLUS
CN 1H-Indene-2-carboxamide, N-(1-methylethyl)-1-(methyloxidoimino)-3-phenyl-6-[2-(2-pyridinyl)ethoxy]-, (1E)- (CA INDEX NAME)

Double bond geometry as shown.



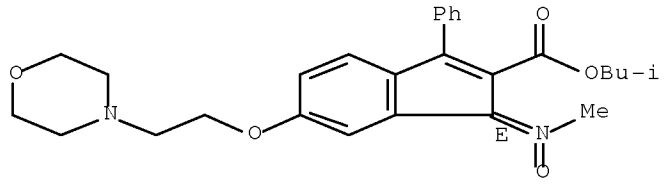
RN 867188-72-5 ZCAPLUS
CN 1H-Indene-2-carboxamide, 6-[2-(5-ethyl-2-pyridinyl)ethoxy]-N-(1-methylethyl)-1-(methyloxidoimino)-3-phenyl-, (1E)- (CA INDEX NAME)

Double bond geometry as shown.



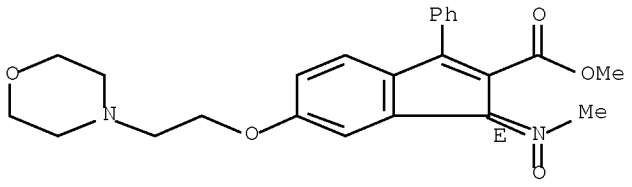
RN 867188-75-8 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-(methyloxidoimino)-6-[2-(4-morpholinyl)ethoxy]-3-phenyl-, 2-methylpropyl ester, (1E)- (CA INDEX NAME)

Double bond geometry as shown.



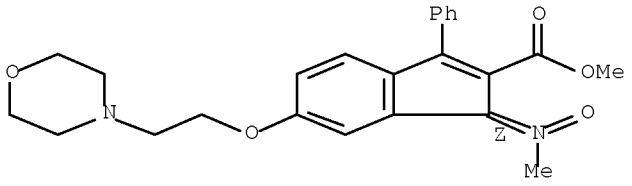
RN 867188-76-9 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-(methyloxidoimino)-6-[2-(4-morpholinyl)ethoxy]-3-phenyl-, methyl ester, (1E)- (CA INDEX NAME)

Double bond geometry as shown.



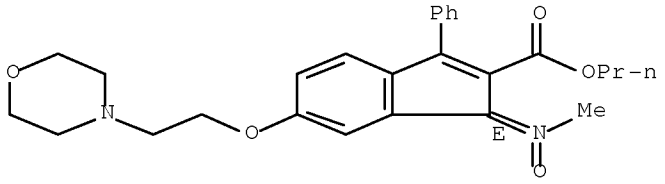
RN 867188-77-0 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-(methyloxidoimino)-6-[2-(4-morpholinyl)ethoxy]-3-phenyl-, methyl ester, (1Z)- (CA INDEX NAME)

Double bond geometry as shown.



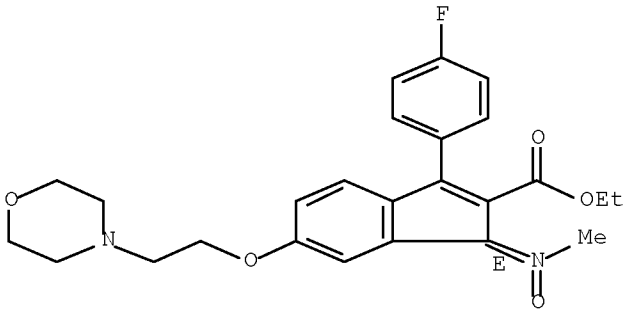
RN 867188-78-1 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-(methyloxidoimino)-6-[2-(4-morpholinyl)ethoxy]-3-phenyl-, propyl ester, (1E)- (CA INDEX NAME)

Double bond geometry as shown.



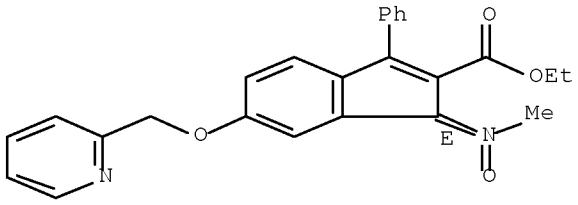
RN 867188-79-2 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 3-(4-fluorophenyl)-1-(methyloxidoimino)-6-[2-(4-morpholinyl)ethoxy]-, ethyl ester, (1E)- (CA INDEX NAME)

Double bond geometry as shown.



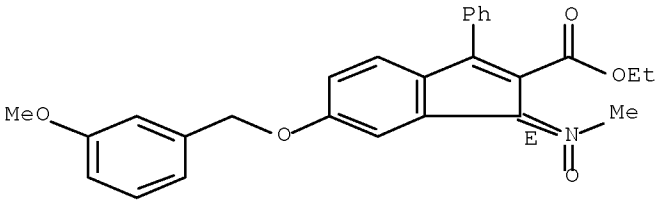
RN 867188-80-5 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-(methyloxidoimino)-3-phenyl-6-(2-pyridinylmethoxy)-, ethyl ester, (1E)- (CA INDEX NAME)

Double bond geometry as shown.



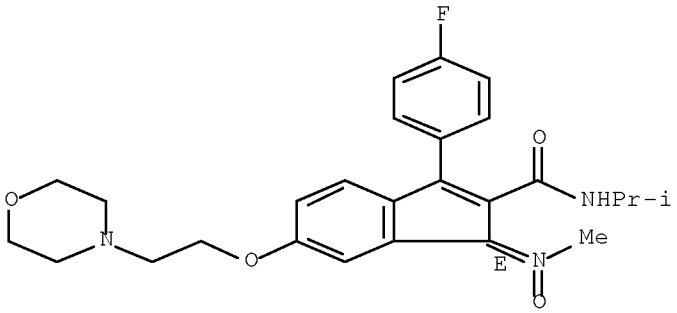
RN 867188-82-7 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 6-[(3-methoxyphenyl)methoxy]-1-(methyloxidoimino)-3-phenyl-, ethyl ester, (1E)- (CA INDEX NAME)

Double bond geometry as shown.



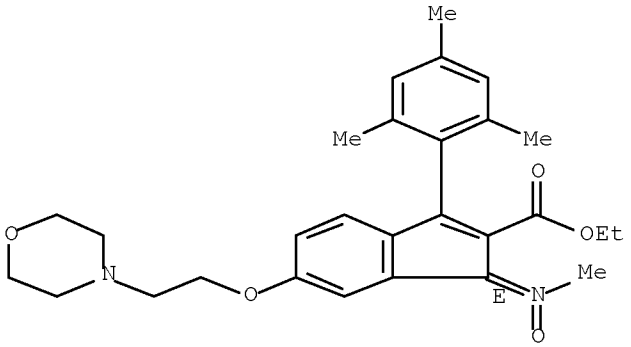
RN 867188-86-1 ZCAPLUS
CN 1H-Indene-2-carboxamide, 3-(4-fluorophenyl)-N-(1-methylethyl)-1-(methyloxidoimino)-6-[2-(4-morpholinyl)ethoxy]-, (1E)- (CA INDEX NAME)

Double bond geometry as shown.



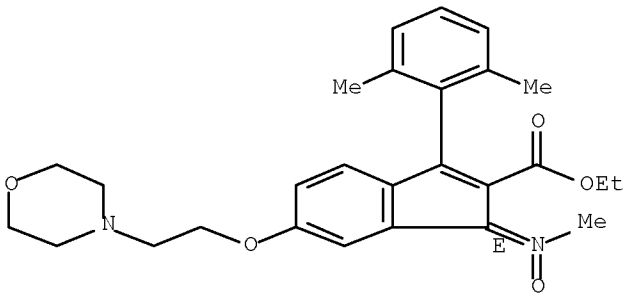
RN 867188-88-3 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-(methyloxidoimino)-6-[2-(4-morpholinyl)ethoxy]-3-(2,4,6-trimethylphenyl)-, ethyl ester, (1E)- (CA INDEX NAME)

Double bond geometry as shown.



RN 867188-89-4 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 3-(2,6-dimethylphenyl)-1-(methyloxidoimino)-6-[2-(4-morpholinyl)ethoxy]-, ethyl ester, (1E)- (CA INDEX NAME)

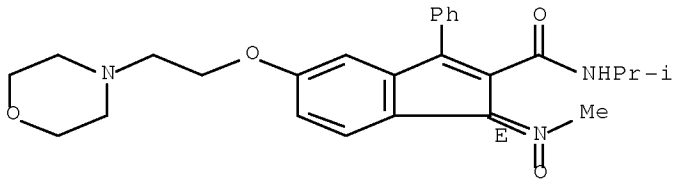
Double bond geometry as shown.



RN 867188-90-7 ZCAPLUS
CN 1H-Indene-2-carboxamide, N-(1-methylethyl)-1-(methyloxidoimino)-5-[2-(4-

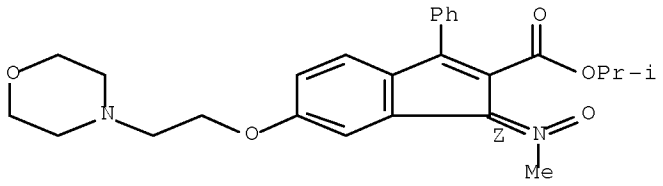
morpholinyl)ethoxy]-3-phenyl-, (1E)- (CA INDEX NAME)

Double bond geometry as shown.



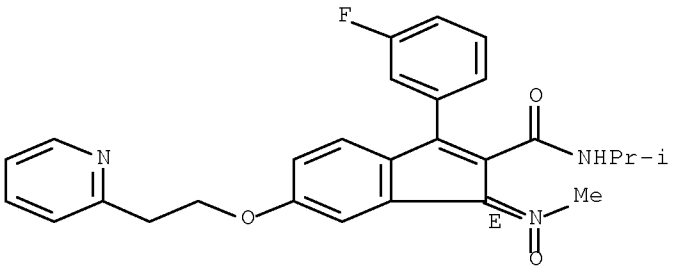
RN 867188-91-8 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-(methyloxidoimino)-6-[2-(4-morpholinyl)ethoxy]-3-phenyl-, 1-methylethyl ester, (1Z)- (CA INDEX NAME)

Double bond geometry as shown.



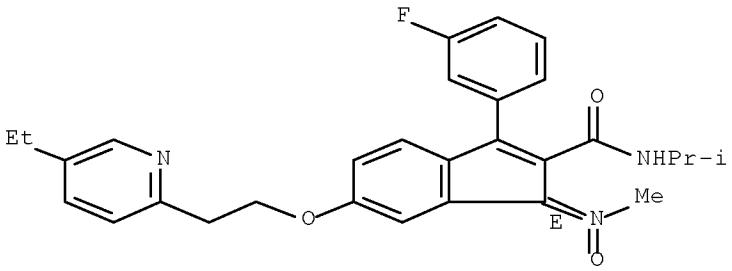
RN 867188-92-9 ZCAPLUS
CN 1H-Indene-2-carboxamide, 3-(3-fluorophenyl)-N-(1-methylethyl)-1-(methyloxidoimino)-6-[2-(2-pyridinyl)ethoxy]-, (1E)- (CA INDEX NAME)

Double bond geometry as shown.



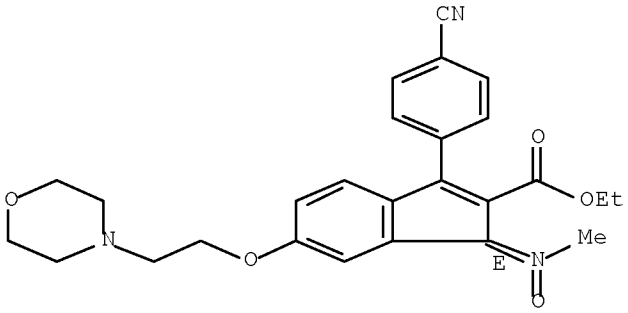
RN 867188-93-0 ZCAPLUS
CN 1H-Indene-2-carboxamide, 6-[2-(5-ethyl-2-pyridinyl)ethoxy]-3-(3-fluorophenyl)-N-(1-methylethyl)-1-(methyloxidoimino)-, (1E)- (CA INDEX NAME)

Double bond geometry as shown.



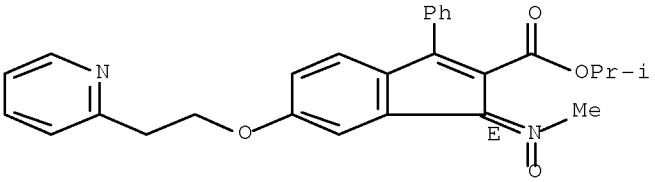
RN 867188-94-1 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 3-(4-cyanophenyl)-1-(methyloxidoimino)-6-[2-(4-morpholinyl)ethoxy]-, ethyl ester, (1E)- (CA INDEX NAME)

Double bond geometry as shown.



RN 867188-95-2 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-(methyloxidoimino)-3-phenyl-6-[2-(2-pyridinyl)ethoxy]-, 1-methylethyl ester, (1E)- (CA INDEX NAME)

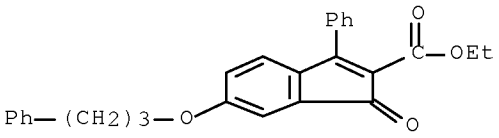
Double bond geometry as shown.



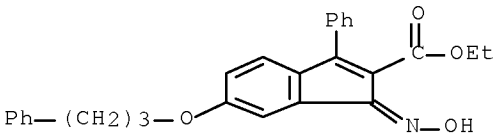
IT 867187-59-5P, 1-Oxo-3-phenyl-6-(3-phenylpropoxy)-1H-indene-2-carboxylic acid ethyl ester 867187-60-8P, 1-Hydroxyimino-3-phenyl-6-(3-phenylpropyloxy)-1H-indene-2-carboxylic acid ethyl ester 867187-62-0P, 3-Phenyl-6-[2-(morpholin-4-yl)ethoxy]-1-oxo-1H-indene-2-carboxylic acid ethyl ester 867187-72-2P, 6-[2-(Morpholin-4-yl)ethoxy]-1-oxo-3-phenyl-1H-indene-2-carboxylic acid isopropylamide 867187-79-9P, 1-Oxo-3-phenyl-6-(3-phenylpropoxy)-1H-indene-2-carbonitrile 867187-80-2P, trans-1-Hydroxyimino-3-phenyl-6-[(3-phenylpropyl)oxy]-1H-indene-2-carbonitrile

867187-88-0P, 6-(Morpholin-4-ylmethyl)-1-oxo-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867187-90-4P, 3-Phenyl-6-(3-phenylpropyloxy)-1-oxo-1H-indene-2-carboxylic acid methyl ester 867187-91-5P, 3-Phenyl-6-(3-phenylpropyloxy)-1-oxo-1H-indene-2-carboxylic acid 867187-92-6P, 3-Phenyl-6-(3-phenylpropyloxy)-1-oxo-1H-indene-2-carboxylic acid cyclohexylamide 867187-94-8P, 2-(Isopropylcarbamoyl)-1-oxo-3-phenyl-1H-inden-5-yl acetate
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 1H-inden-1-imine N-oxides as selective modulators of peroxisome proliferator activated receptors)

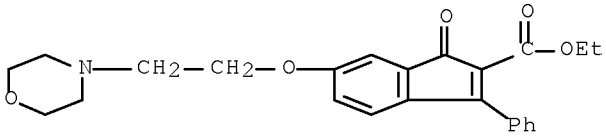
RN 867187-59-5 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-oxo-3-phenyl-6-(3-phenylpropoxy)-, ethyl ester (CA INDEX NAME)



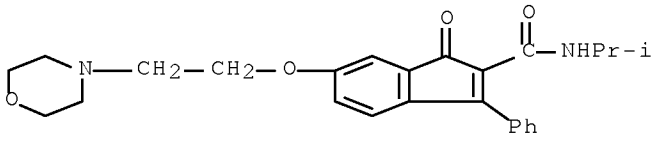
RN 867187-60-8 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-(hydroxyimino)-3-phenyl-6-(3-phenylpropoxy)-, ethyl ester (CA INDEX NAME)



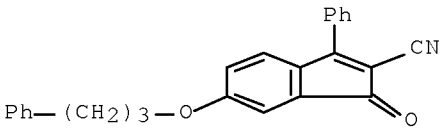
RN 867187-62-0 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 6-[2-(4-morpholinyl)ethoxy]-1-oxo-3-phenyl-, ethyl ester (CA INDEX NAME)



RN 867187-72-2 ZCAPLUS
CN 1H-Indene-2-carboxamide, N-(1-methylethyl)-6-[2-(4-morpholinyl)ethoxy]-1-oxo-3-phenyl- (CA INDEX NAME)

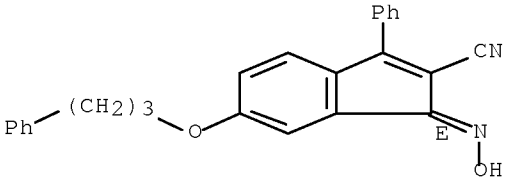


RN 867187-79-9 ZCAPLUS
CN 1H-Indene-2-carbonitrile, 1-oxo-3-phenyl-6-(3-phenylpropoxy)- (CA INDEX NAME)

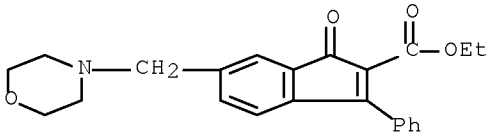


RN 867187-80-2 ZCAPLUS
CN 1H-Indene-2-carbonitrile, 1-(hydroxyimino)-3-phenyl-6-(3-phenylpropoxy)-, (1E)- (CA INDEX NAME)

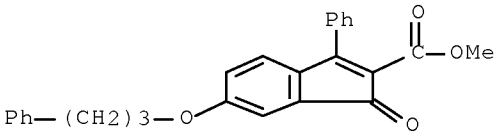
Double bond geometry as shown.



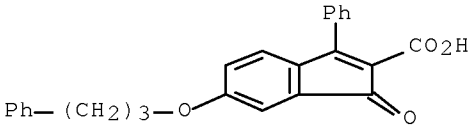
RN 867187-88-0 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 6-(4-morpholinylmethyl)-1-oxo-3-phenyl-, ethyl ester (CA INDEX NAME)



RN 867187-90-4 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-oxo-3-phenyl-6-(3-phenylpropoxy)-, methyl ester (CA INDEX NAME)



RN 867187-91-5 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-oxo-3-phenyl-6-(3-phenylpropoxy)- (CA INDEX NAME)



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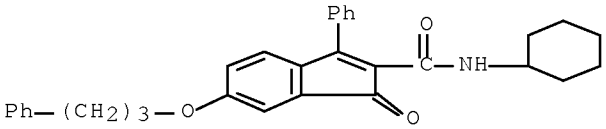
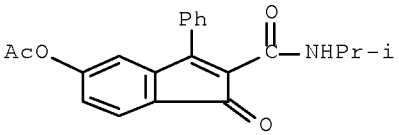


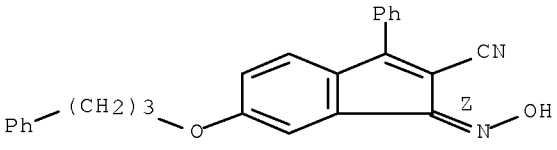
RN 867187-94-8 ZCAPLUS
CN 1H-Indene-2-carboxamide, 5-(acetyloxy)-N-(1-methylethyl)-1-oxo-3-phenyl- (CA INDEX NAME)



IT 867187-81-3P, cis-1-Hydroxyimino-3-phenyl-6-[(3-phenylpropyl)oxy]-1H-indene-2-carbonitrile 867187-82-4P, 1-(trans-Methoxyimino)-3-phenyl-6-(3-phenylpropoxy)-1H-indene-2-carbonitrile
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of 1H-inden-1-imine N-oxides as selective modulators of peroxisome proliferator activated receptors)
RN 867187-81-3 ZCAPLUS

CN 1H-Indene-2-carbonitrile, 1-(hydroxyimino)-3-phenyl-6-(3-phenylpropoxy)-, (1Z)- (CA INDEX NAME)

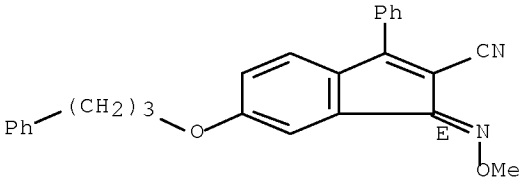
Double bond geometry as shown.



RN 867187-82-4 ZCAPLUS

CN 1H-Indene-2-carbonitrile, 1-(methoxyimino)-3-phenyl-6-(3-phenylpropoxy)-, (1E)- (CA INDEX NAME)

Double bond geometry as shown.



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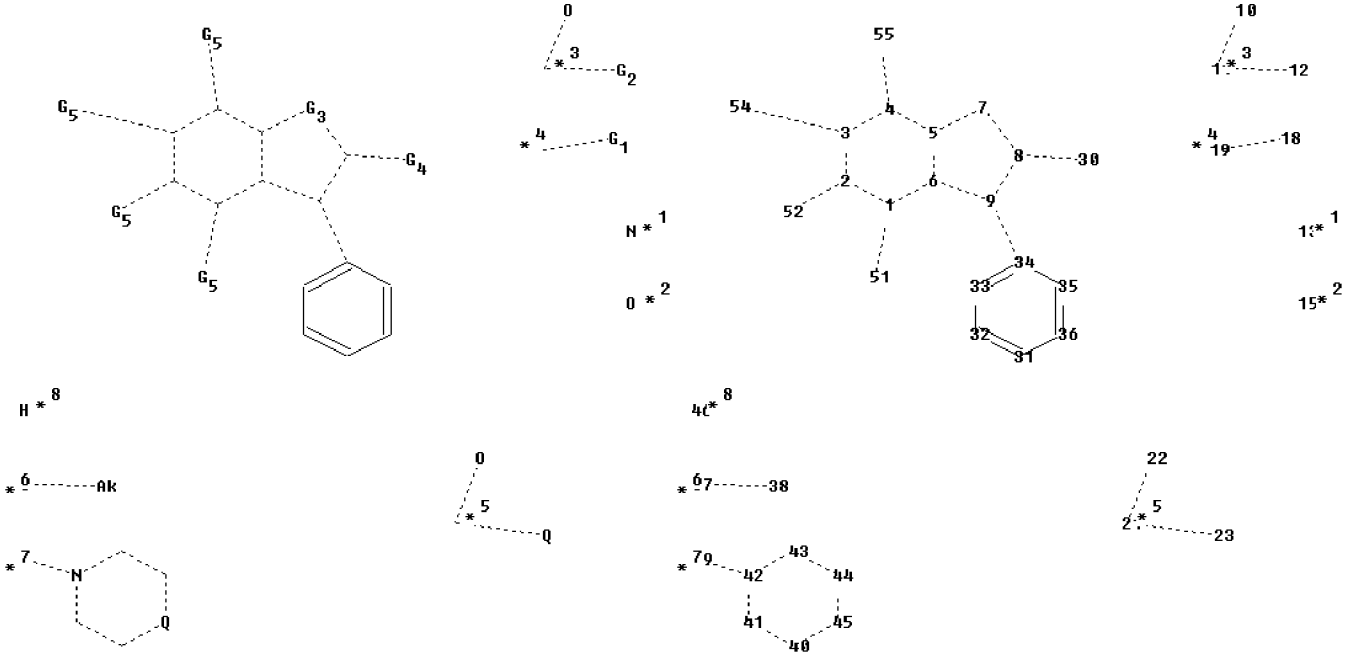

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ring nodes :
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ring/chain nodes :
13
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chain bonds :
1-51  2-52  3-54  4-55  8-30  9-34  10-11  11-12  18-19  21-22  21-23  37-38  39-42

ring bonds :
1-2  1-6  2-3  3-4  4-5  5-6  5-7  6-9  7-8  8-9  31-32  31-36  32-33  33-34  34-35
35-36  40-41  40-45  41-42  42-43  43-44  44-45
exact/norm bonds :
1-2  1-6  1-51  2-3  2-52  3-4  3-54  4-5  4-55  5-6  5-7  6-9  7-8  8-9  8-30  9-
34
10-11  11-12  18-19  21-22  21-23  37-38  39-42  40-41  40-45  41-42  42-43  43-44
44-45
normalized bonds :
31-32  31-36  32-33  33-34  34-35  35-36


G1:[*1],[*2]

G2:Cb,Ak

G3:[*3],[*4]

G4:CN,[*5]

G5:[*6],[*7],[*8]

Connectivity :
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Match level :
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11:Atom  12:CLASS  13:CLASS  15:CLASS  18:CLASS  19:Atom  21:CLASS  22:CLASS
23:CLASS  30:CLASS
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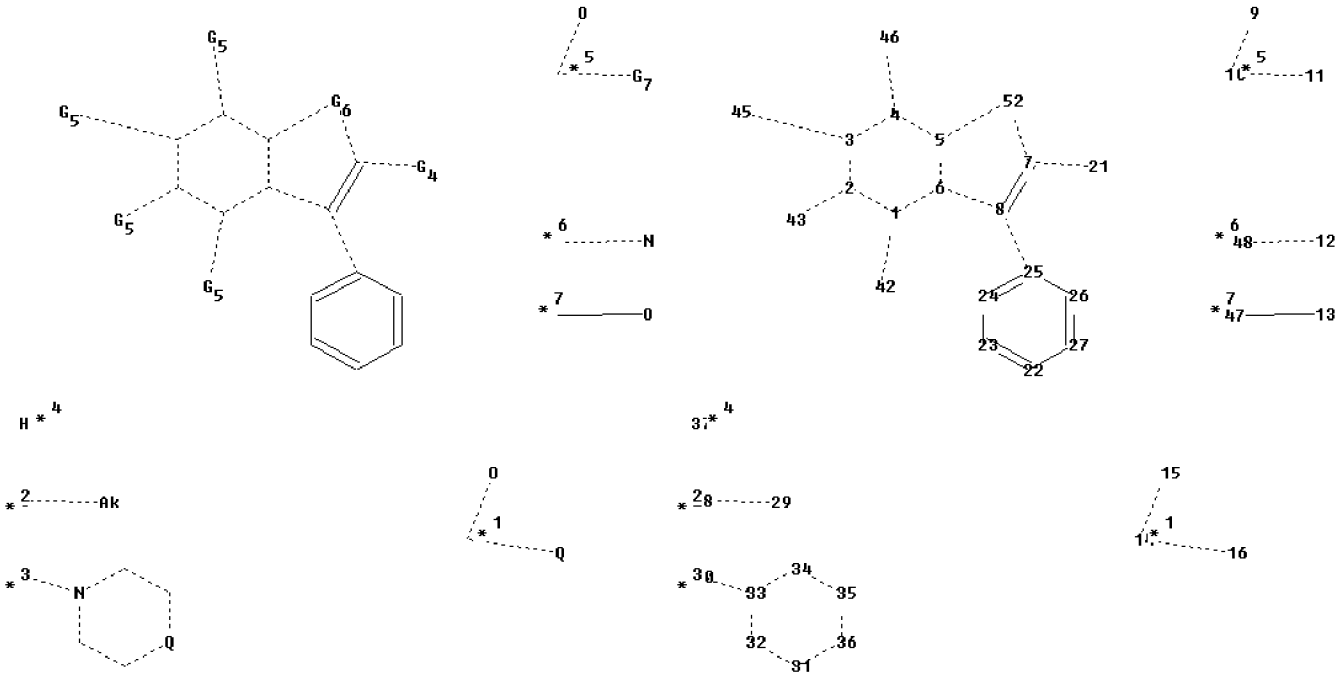

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ring nodes :
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52
ring/chain nodes :
12
chain bonds :
1-42 2-43 3-45 4-46 7-21 8-25 9-10 10-11 12-48 13-47 14-15 14-16 28-29
30-33
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-52 6-8 7-8 7-52 22-23 22-27 23-24 24-25 25-
26
26-27 31-32 31-36 32-33 33-34 34-35 35-36
exact/norm bonds :
1-2 1-6 1-42 2-3 2-43 3-4 3-45 4-5 4-46 5-6 5-52 6-8 7-21 7-8 7-52
8-25 9-10 10-11 12-48 13-47 14-15 14-16 28-29 30-33 31-32 31-36 32-33
33-34 34-35 35-36

normalized bonds :
22-23 22-27 23-24 24-25 25-26 26-27

G4:CN,[*1]

G5:[*2],[*3],[*4]

G6:[*5],[*6],[*7]

G7:Cb,Ak

Connectivity :
14:3 E exact RC ring/chain 15:1 E exact RC ring/chain
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:CLASS 10:Atom
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 21:CLASS 22:Atom

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23:Atom  24:Atom  25:Atom
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52:CLASS



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FILE COVERS 1907 - 23 Jun 2008  VOL 148 ISS 26
FILE LAST UPDATED: 22 Jun 2008  (20080622/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

  This file contains CAS Registry Numbers for easy and accurate
  substance identification.
'OBI' IS DEFAULT SEARCH FIELD FOR 'ZCAPLUS' FILE

=> d stat que L32
L4            82 SEA FILE=REGISTRY ABB=ON  PLU=ON  (100-46-9/BI OR 100-52-7/BI
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                  OR 94-02-0/BI)
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L5              STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -  AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.
L7          427 SEA FILE=REGISTRY SSS FUL L5
L8           45 SEA FILE=REGISTRY ABB=ON  PLU=ON  L4 AND L7
L25             STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -  AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.
L27         166 SEA FILE=REGISTRY SUB=L7 SSS FUL L25
L29          37 SEA FILE=REGISTRY ABB=ON  PLU=ON  L27 AND L8
L32           6 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  L29


=> d stat que L77
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                  OR 94-02-0/BI)
L5              STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -  AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.
L7          427 SEA FILE=REGISTRY SSS FUL L5
L8           45 SEA FILE=REGISTRY ABB=ON  PLU=ON  L4 AND L7
L25             STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -  AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.
L27         166 SEA FILE=REGISTRY SUB=L7 SSS FUL L25
L29          37 SEA FILE=REGISTRY ABB=ON  PLU=ON  L27 AND L8
L32           6 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  L29
L54      171149 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  ?DIABET?/BI
L55       56841 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  OBES?/BI
L56       11261 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  ANTIOBES?/BI
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L59      225556 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  ?INSULIN?/BI
L60      124786 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  ?HYPERTENS?/BI
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L75       39743 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  ?MELANOM?/BI
L76       51481 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  ?ANGIOGEN?/BI
L77           5 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  L32 AND (L54 OR L55 OR L56 OR
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=> d stat que L80
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                 OR 94-02-0/BI)
L5              STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -  AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.
L7           427 SEA FILE=REGISTRY SSS FUL L5
L8            45 SEA FILE=REGISTRY ABB=ON  PLU=ON  L4 AND L7
L25             STR
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* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -  AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.
L27         166 SEA FILE=REGISTRY SUB=L7 SSS FUL L25
L29          37 SEA FILE=REGISTRY ABB=ON  PLU=ON  L27 AND L8
L32           6 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  L29
L78       11482 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  PPAR/BI
L79       23760 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  PEROXISOM?/BI
L80           5 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  L32 AND (L78 OR L79)


=> s (L32 or L77 or L80 ) not L101
L102          3 (L32 OR L77 OR L80 ) NOT L101

=> d ibib abs hitind hitstr L102 1-3

L102 ANSWER 1 OF 3  ZCAPLUS  COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER:         2008:411947  ZCAPLUS  Full-text
DOCUMENT NUMBER:          148:427397
TITLE:                    Novel polybenzofulvene derivatives, synthesis and uses
                          thereof
INVENTOR(S):              Cappelli, Andrea; Galeazzi, Simone; Anzini, Maurizio;
                          Vomero, Salvatore
PATENT ASSIGNEE(S):       Universita Degli Studi di Siena, Italy
SOURCE:                   PCT Int. Appl., 47pp.
                          CODEN: PIXXD2
DOCUMENT TYPE:            Patent
LANGUAGE:                 English
FAMILY ACC. NUM. COUNT:   1
PATENT INFORMATION:

     PATENT NO.           KIND   DATE        APPLICATION NO.         DATE
     ---------------      ----   --------    --------------------    --------
     WO 2008037604         A1    20080403    WO 2007-EP59698         20070914
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             GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG,
             KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LY, MA, MD, ME,
             MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL,
             PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN,
             TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW
         RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,
             IS, IT, LT, LU, LV, MC, MT, NL, PL, PT, RO, SE, SI, SK, TR, BF,
             BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW,
             GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ,
             BY, KG, KZ, MD, RU, TJ, TM
PRIORITY APPLN. INFO.:                       US 2006-846915P     P  20060925
OTHER SOURCE(S):          CASREACT 148:427397
GI
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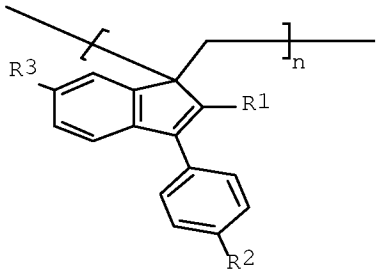


I

AB The present invention relates to polymers of formula poly-3 (I), their synthesis, intermediates and uses thereof; wherein R1 is H, CH3, CN, a halogen, COOR; R = H, a C1-5 alkyl group, or -(CH2-CH2O)m-CH3, a substituted ethynyl group, or an alkyl group; m is 3-15; R2 and R3 represent a hydrogen atom, a halogen atom, an alkyl group or a hydroxyl group; n is 1-10,000. The invention also related to a pharmaceutical formulation comprising the polymer as drug controlled release pharmaceutical formulation.

CC 35-4 (Chemistry of Synthetic High Polymers)
Section cross-reference(s): 63

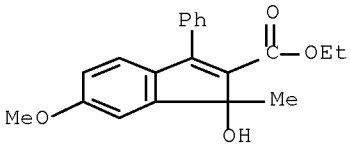
IT 6048-68-6P, Nonaethylene glycolmono methyl ether 13093-22-6P, 2-Chloro-3-phenyl-1H-1-indenone 13304-52-4P, 2-Methyl-3-phenyl-1H-1-indenone 19772-61-3P, 2-Bromo-3-phenyl-1H-1-indenone 35491-56-6P, 1-Oxo-3-phenyl-1H-2-indenecarbonitrile 41916-15-8P, 3-Phenyl-1H-1-indenone 72593-77-2P, 1-Bromo-2-(2-(2-methoxyethoxy)ethoxy)ethane 94224-67-6P, Ethyl 1-Oxo-3-phenyl-1H-2-indenecarboxylate 150192-43-1P, 3-Phenyl-2-(trimethylsilyl)-1H-1-indenone 168007-89-4P, 1-Methylene-3-phenyl-1H-indene 222041-22-7P, 1,2-Dimethyl-3-phenyl-1H-1-indenol 696661-22-0P, 3-(4-Methylphenyl)-1-oxo-1H-2-indenecarbonitrile 724776-29-8P, Ethyl 1-Hydroxy-1-methyl-3-phenyl-1H-indene-2-carboxylate 850209-49-3P, Ethyl 6-methoxy-1-oxo-3-phenyl-1H-indene-2-carboxylate 867214-96-8P, Ethyl 1-Hydroxy-1-methyl-6-methoxy-3-phenyl-1H-indene-2-carboxylate 937079-93-1P, Ethyl (Z)-2-cyano-3-(4-methylphenyl)-3-phenyl-2-propenoate 937079-95-3P, (E)-2-Cyano-3-(4-methylphenyl)-3-phenyl-2-propenoic acid 937079-96-4P, (Z)-2-Cyano-3-(4-methylphenyl)-3-phenyl-2-propenoic acid 937079-97-5P, 6-Methyl-1-oxo-3-phenyl-1H-2-indenecarbonitrile 937079-98-6P, 3-Phenyl-2-[2-(2-pyridyl)-1-ethynyl]-1H-1-indenone 937080-00-7P, 1-Methyl-3-phenyl-1H-1-indenol 937080-01-8P, 1-Methyl-3-phenyl-2-(trimethylsilyl)-1H-1-indenol 937080-02-9P, 2-Chloro-1-methyl-3-phenyl-1H-1-indenol 937080-04-1P, 2-Bromo-1-methyl-3-phenyl-1H-1-indenol 937080-09-6P, 1-Hydroxy-1-methyl-3-(4-methylphenyl)-1H-indene-2-carbonitrile 937080-10-9P, 1,6-Dimethyl-1-hydroxy-3-phenyl-1H-indene-2-carbonitrile 937080-11-0P, 1-Methyl-3-phenyl-2-2-(2-pyridyl)-1-ethynyl]-1H-1-indenol 937080-18-7P, 2-Fluoro-1-methyl-3-phenyl-1H-1-indenol 937080-19-8P, 2-Fluoro-1-methylene-3-phenyl-1H-indene 937080-20-1P, 2-Chloro-1-methylene-3-phenyl-1H-indene 937080-21-2P, 2-Bromo-1-methylene-3-phenyl-1H-indene 937080-22-3P, 2-Methyl-1-methylene-3-phenyl-1H-indene 937080-23-4P, 1-Methylene-3-phenyl-1H-indene-2-carbonitrile 937080-24-5P, 1-Methylene-3-(4-methylphenyl)-1H-indene-2-carbonitrile 937080-25-6P, 6-Methyl-1-methylene-3-phenyl-1H-indene-2-carbonitrile 937080-26-7P, Ethyl 1-methylene-3-phenyl-1H-indene-2-carboxylate 937080-32-5P, 1-Methylene-3-phenyl-2-[2-(2-pyridyl)-1-ethynyl]-1H-indene 1016567-36-4P, 2-[2-(2-Methoxyethoxy)ethoxyl]ethyl 3-(4-Methylphenyl)-1-

oxo-1H-indene-2-carboxylate 1016567-41-1P 1016567-46-6P, [2-[2-(2-Methoxyethoxy)ethoxyl]ethyl 1-Hydroxy-1-methyl-3-(4-methylphenyl)-1H-indene-2-carboxylate 1016567-48-8P, 2,5,8,11,14,17,20,23,26-Nonaoxaoctacosan-28-yl 1-hydroxy-1-methyl-3-(4-methylphenyl)-1H-indene-2-carboxylate 1016567-53-5P, [2-[2-(2-Methoxyethoxy)ethoxy]ethyl 1-Methylene-3-(4-methylphenyl)-1H-indene-2-carboxylate 1016567-55-7P, 2,5,8,11,14,17,20,23,26-Nonaoxaoctacosan-28-yl 1-methylene-3-(4-methylphenyl)-1H-indene-2-carboxylate 1016567-57-9P, Ethyl 1-Methylene-6-methoxy-3-phenyl-1H-indene-2-carboxylate
RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(production of polybenzofulvene derivs. for pharmaceutical formulation)

IT 867214-96-8P, Ethyl 1-Hydroxy-1-methyl-6-methoxy-3-phenyl-1H-indene-2-carboxylate
RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(production of polybenzofulvene derivs. for pharmaceutical formulation)

RN 867214-96-8 ZCAPLUS

CN 1H-Indene-2-carboxylic acid, 1-hydroxy-6-methoxy-1-methyl-3-phenyl-, ethyl ester (CA INDEX NAME)



REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L102 ANSWER 2 OF 3 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2007:1388077 ZCAPLUS Full-text

TITLE: Pharmacophore modeling and parallel screening for PPAR ligands

AUTHOR(S): Markt, Patrick; Schuster, Daniela; Kirchmair, Johannes; Laggner, Christian; Langer, Thierry

CORPORATE SOURCE: Department of Pharmaceutical Chemistry, Institute of Pharmacy and Center for Molecular Biosciences Innsbruck (CMBI), University of Innsbruck, Innsbruck, 6020, Austria

SOURCE: Journal of Computer-Aided Molecular Design (2007), 21(10-11), 575-590
CODEN: JCADEQ; ISSN: 0920-654X

PUBLISHER: Springer

DOCUMENT TYPE: Journal

LANGUAGE: English

AB We describe the generation and validation of pharmacophore models for PPARs, as well as a large scale validation of the parallel screening approach by screening PPAR ligands against a large database of structure-based models. A large test set of 357 PPAR ligands was screened against 48 PPAR models to determine the best models for agonists of PPAR-α, PPAR-δ, and PPAR-γ. Afterwards, a parallel screen was performed using the 357 PPAR ligands and 47 structure-based models for PPARs, which were integrated into a 1537 models comprising inhouse pharmacophore database, to assess the enrichment of PPAR ligands within the PPAR hypotheses. For these purposes, we categorized the

1537 database models into 181 protein targets and developed a score that ranks the retrieved targets for each ligand. Thus, we tried to find out if the concept of parallel screening is able to predict the correct pharmacol. target for a set of compds. The PPAR target was ranked first more often than any other target. This confirms the ability of parallel screening to forecast the pharmacol. active target for a set of compds.

CC 1-3 (Pharmacology)
Section cross-reference(s): 6

ST peroxisome proliferator activated receptor ligand structure virtual screening pharmacophore

IT Structure-activity relationship
(antidiabetic; pharmacophore modeling and parallel screening for PPAR ligands)

IT Structure-activity relationship
(hypolipemic; pharmacophore modeling and parallel screening for PPAR ligands)

IT Antidiabetic agents
Antiobesity agents
Diabetes mellitus
Drug targets
Hyperlipidemia
Hypolipemic agents
Molecular association
Molecular modeling
Obesity
Pharmacophores
(pharmacophore modeling and parallel screening for PPAR ligands)

IT Peroxisome proliferator-activated receptors
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(pharmacophore modeling and parallel screening for PPAR ligands)

IT Structure-activity relationship
(receptor-binding; pharmacophore modeling and parallel screening for PPAR ligands)

IT Drug screening
(virtual; pharmacophore modeling and parallel screening for PPAR ligands)

IT Peroxisome proliferator-activated receptors
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(α; pharmacophore modeling and parallel screening for PPAR ligands)

IT Peroxisome proliferator-activated receptors
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(γ; pharmacophore modeling and parallel screening for PPAR ligands)

IT Peroxisome proliferator-activated receptors
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(δ; pharmacophore modeling and parallel screening for PPAR ligands)

IT 637-07-0 882-09-7 1002-84-2 1191-85-1 5490-93-7 7668-58-8
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50892-23-4 79558-09-1 96207-25-9 122320-47-2 122320-74-5
133397-73-6 135133-49-2 142696-28-4 159017-08-0 178610-09-8
185679-07-6 185679-34-9 194608-80-5 196808-14-7 218600-44-3
219653-35-7 219653-36-8 219653-78-8 219654-01-0 219654-02-1
219654-03-2 227002-04-2 229980-32-9 229980-36-3 229980-37-4
229980-39-6 229980-40-9 229980-46-5 236393-35-4 265301-05-1
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RL: PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(pharmacophore modeling and parallel screening for PPAR ligands)

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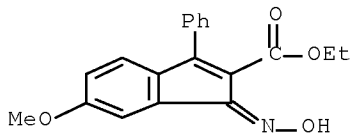
RL: PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(pharmacophore modeling and parallel screening for PPAR ligands)

IT 867215-17-6
RL: PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(pharmacophore modeling and parallel screening for PPAR ligands)

RN 867215-17-6 ZCAPLUS

CN 1H-Indene-2-carboxylic acid, 1-(hydroxyimino)-6-methoxy-3-phenyl-, ethyl ester (CA INDEX NAME)



REFERENCE COUNT: 46 THERE ARE 46 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L102 ANSWER 3 OF 3 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2005:1154511 ZCAPLUS Full-text
DOCUMENT NUMBER: 143:405636
TITLE: Preparation of indenes as selective modulators of peroxisome proliferator activated receptors
PATENT ASSIGNEE(S): Korea Research Institute of Chemical Technology, S. Korea; Jeil Pharm. Co., Ltd.; Korea Research Institute of Bioscience and Biotechnology; Cj Corp.; Cheon, Hyae Gyeong; Yoo, Sung-Eun; Kim, Sung Soo; Yang, Sung-Don; Kim, Kwang-Rok; et al.
SOURCE: PCT Int. Appl., 63 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005100297	A1	20051027	WO 2005-KR1051	20050412

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML,

	MR, NE, SN, TD, TG				
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AU 2005233038		A1	20051027	AU 2005-233038	20050412
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EP 1756036		A1	20070228	EP 2005-733516	20050412
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BR 2005009869		A	20071016	BR 2005-9869	20050412
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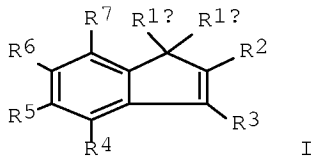
MX 2006PA11514		A	20070802	MX 2006-PA11514	20061005
US 20070225288		A1	20070927	US 2006-599913	20061023
IN 2006DN06489		A	20070831	IN 2006-DN6489	20061102
PRIORITY APPLN. INFO.:				KR 2004-25218 A	20040413
				WO 2005-KR1051 W	20050412

OTHER SOURCE(S): CASREACT 143:405636; MARPAT 143:405636

GI



I

AB The inventive indenes (shown as I; variables defined below; e.g. 1-hydroxy-6-methoxy-1,3-diphenyl-1H-indene-2-carboxylic acid Et ester (II)) are capable of selectively modulating the activities of peroxisome proliferator activated receptors (PPARs), causing no adverse side effects, and thus, they are useful for the treatment and prevention of disorders modulated by PPARs, i.e., metabolic syndromes such as diabetes, obesity, arteriosclerosis, hyperlipidemia, hyperinsulinism and hypertension, inflammatory diseases such as osteoporosis, liver cirrhosis and asthma, and cancer. Methods of preparation are claimed and .apprx.30 example prepns. are included. For example, II was prepared in 2 steps (72 and 76 % yields) by oxidation of 6-methoxy-3-phenyl-1H-indene-2-carboxylic acid Et ester (preparation given) with SeO2 to give 6-methoxy-1-oxo-3-phenyl-1H-indene-2-carboxylic acid Et ester, which was reacted with phenylmagnesium chloride. EC50 values for activation of PPARγ are tabulated for 15 examples of I; they exhibited superior activation over rosiglitazone. 1-Hydroxy-6-[2- (morpholin-4-yl)ethoxy]-1,3-diphenyl-1H-indene-2-carboxylic acid Et ester hydrochloride was tested for effectiveness in lowering blood glucose level in ob/ob mice; it has an excellent effect in lowering both blood glucose and insulin levels, when it is administered by either orally or i.p. with no side effects such as weight gain, hepatotoxicity or cardiotoxicity. For I: R1a is OH or H; R1b is C1-6 alkyl, C3-6 cycloalkyl, benzyl or Ph ((un)substituted with ≥1 halogen, CN, NH2, NO2 and ORa), when R1a is OH; when R1a is H, R1b is ORa, NRbRc, NHCORa, morpholino, thiomorpholino, or 4-Rapiperazino; R2 is CN, CO2Ra or CONReRf; R3 is Ph (un)substituted with ≥1 halogen, CN, NH2, NO2, ORa and C1-6 alkyl; and R4, R5, R6 and R7 = H, O(CH2)mRg or CH2Rh; in which Ra is H, C1-6 alkyl or C3-6 cycloalkyl, the C1-6 alkyl and C3-6 cycloalkyl being (un)substituted with ≥1 halogens; Rb, Rc, Re and Rf = H, C1-6 alkyl, C3-6 cycloalkyl or benzyl; Rg is H, Ra-substituted pyridinyl, morpholino, thiomorpholino, 4-Rapiperazino, or

Ph, the Ph being (un)substituted with ≥1 halogen, CN, NH2 and NO2; Rh is morpholino, thiomorpholino, or 4-Rapiperazino; and m = 1-3.

IC ICM C07C069-753

CC 24-7 (Alicyclic Compounds)
Section cross-reference(s): 1, 2, 63

ST indene prepn selective modulator peroxisome proliferator activated receptor

IT Heart
Liver
(lack of toxicity of potential drug; preparation of indenes as selective modulators of peroxisome proliferator activated receptors)

IT Cardiotoxicity
Drug toxicity
Hepatotoxicity
(lack of; preparation of indenes as selective modulators of peroxisome proliferator activated receptors)

IT Peroxisome proliferator-activated receptors
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(modulators; preparation of indenes as selective modulators of peroxisome proliferator activated receptors)

IT Antiarteriosclerotics
Antiasthmatics
Antidiabetic agents
Antihypertensives
Antiobesity agents
Antitumor agents
Arteriosclerosis
Asthma
Cirrhosis
Diabetes mellitus
Drug delivery systems
Human
Hypertension
Hypolipemic agents
Neoplasm
Obesity
Osteoporosis
Hyperlipidemia
RL: BIOL (Biological study)
(preparation of indenes as selective modulators of peroxisome proliferator activated receptors)

IT Peroxisome proliferator-activated receptors
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(γ, modulators; preparation of indenes as selective modulators of peroxisome proliferator activated receptors)

IT 867214-93-5P, 1-Hydroxy-6-methoxy-1,3-diphenyl-1H-indene-2-carboxylic acid ethyl ester 867214-96-8P, 1-Hydroxy-6-methoxy-1-methyl-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867214-97-9P, 1-Benzyl-1-hydroxy-6-methoxy-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867214-98-0P, 1-Cyclohexyl-1-hydroxy-6-methoxy-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867214-99-1P, 1-Hydroxy-1,3-diphenyl-6-(3-phenylpropoxy)-1H-indene-2-carboxylic acid ethyl ester 867215-16-5P, 1-Amino-6-methoxy-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867215-18-7P, 1-Amino-3-phenyl-6-(3-phenylpropoxy)-1H-indene-2-carboxylic acid ethyl ester 867215-19-8P, 1-Amino-6-[2-(morpholin-4-yl)ethoxy]-3-phenyl-1H-indene-2-carboxylic acid cyclohexylamide
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(drug candidate; preparation of indenes as selective modulators of peroxisome proliferator activated receptors)

IT 867187-97-1P, 1-Hydroxy-6-[2-(morpholin-4-yl)ethoxy]-1,3-diphenyl-1H-indene-2-carboxylic acid ethyl ester hydrochloride 867214-94-6P, 1-Hydroxy-6-methoxy-1-(3-methoxyphenyl)-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867214-95-7P, 1-Hydroxy-1-isopropyl-6-methoxy-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867215-00-7P, 1-Hydroxy-6-[2-(morpholin-4-yl)ethoxy]-1,3-diphenyl-1H-indene-2-carboxylic acid ethyl ester 867215-01-8P, 1-Hydroxy-6-[(morpholin-4-yl)methyl]-1,3-diphenyl-1H-indene-2-carboxylic acid ethyl ester 867215-02-9P, 1-Hydroxy-1,3-diphenyl-6-[2-(pyridin-2-yl)ethoxy]-1H-indene-2-carboxylic acid ethyl ester 867215-04-1P, 1-Hydroxy-1,3-diphenyl-6-(3-phenylpropoxy)-1H-indene-2-carbonitrile 867215-07-4P, 1-Hydroxy-1,3-diphenyl-6-(3-phenylpropoxy)-1H-indene-2-carboxylic acid methyl ester 867215-08-5P, 1-Hydroxy-6-methoxy-1,3-diphenyl-1H-indene-2-carboxylic acid 867215-09-6P, 1-Hydroxy-6-methoxy-1-methyl-3-phenyl-1H-indene-2-carboxylic acid 867215-10-9P, 1-Benzyl-1-hydroxy-6-methoxy-3-phenyl-1H-indene-2-carboxylic acid 867215-11-0P, 1-Hydroxy-1,3-diphenyl-6-(3-phenylpropoxy)-1H-indene-2-carboxylic acid 867215-12-1P, 1-Cyclohexyl-1-hydroxy-6-methoxy-3-phenyl-1H-indene-2-carboxylic acid 867215-13-2P, 1,6-Dimethoxy-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867215-15-4P, 1-Ethoxy-6-methoxy-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867215-25-6P, 1-Amino-3-phenyl-6-(3-phenylpropoxy)-1H-indene-2-carbonitrile 867215-27-8P, 1-Acetylamino-6-methoxy-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867215-28-9P, 6-Methoxy-3-phenyl-1-propionylamino-1H-indene-2-carboxylic acid ethyl ester 867215-29-0P, 1-Acetylamino-3-phenyl-6-(3-phenylpropoxy)-1H-indene-2-carboxylic acid ethyl ester 867215-30-3P, 1-Acetylamino-6-[2-(morpholin-4-yl)ethoxy]-3-phenyl-1H-indene-2-carboxylic acid cyclohexylamide 867215-31-4P, 1-Diethylamino-6-methoxy-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867215-32-5P, 1-Ethylamino-6-methoxy-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867215-33-6P, 6-Methoxy-1-(morpholin-4-yl)-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867215-34-7P, 1-Benzylamino-6-methoxy-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867215-35-8P, 1-Cyclohexylamino-6-methoxy-3-phenyl-1H-indene-2-carboxylic acid ethyl ester
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of indenes as selective modulators of peroxisome proliferator activated receptors)

IT 9004-10-8, Insulin, biological studies
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(hyperinsulinemia; preparation of indenes as selective modulators of peroxisome proliferator activated receptors)

IT 94-02-0, Ethyl benzoylacetate 100-46-9, Benzylamine, reactions 100-52-7, Benzaldehyde, reactions 100-59-4, Phenylmagnesium chloride 103-74-2, 2-Pyridineethanol 105-58-8, Diethyl carbonate 108-91-8, Cyclohexylamine, reactions 109-89-7, Diethylamine, reactions 110-91-8, Morpholine, reactions 585-74-0 622-40-2, 4-(2-Hydroxyethyl)morpholine 637-59-2, 1-Bromo-3-phenylpropane 824-98-6, 3-Methoxybenzyl chloride 931-51-1, Cyclohexylmagnesium chloride 1068-55-9, Isopropylmagnesium chloride 6921-34-2, Benzylmagnesium chloride 36282-40-3, 3-Methoxyphenylmagnesium bromide 60760-06-7, 3-Chloromethylphenol 867187-77-7, 3-Phenyl-1-[3-(3-phenylpropoxy)phenyl]-2-propen-1-one
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of indenes as selective modulators of peroxisome

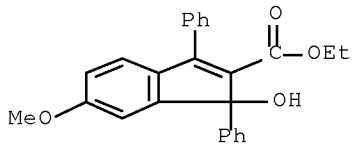
proliferator activated receptors)

IT 33166-79-9P, 3-Oxo-3-(m-tolyl)propionic acid ethyl ester 850209-49-3P, 6-Methoxy-1-oxo-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867187-56-2P, 2-(3-Hydroxybenzyl)-3-oxo-3-phenylpropionic acid ethyl ester 867187-57-3P, 6-Hydroxy-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867187-58-4P, 6-Hydroxy-1-oxo-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867187-59-5P, 1-Oxo-3-phenyl-6-(3-phenylpropoxy)-1H-indene-2-carboxylic acid ethyl ester 867187-60-8P, 1-Hydroxyimino-3-phenyl-6-(3-phenylpropoxy)-1H-indene-2-carboxylic acid ethyl ester 867187-62-0P, 6-[2-(Morpholin-4-yl)ethoxy]-1-oxo-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867187-79-9P, 1-Oxo-3-phenyl-6-(3-phenylpropoxy)-1H-indene-2-carbonitrile 867187-84-6P, 2-(3-Methylbenzoyl)-3-phenylacrylic acid ethyl ester 867187-85-7P, 5-Methyl-3-oxo-1-phenylindane-2-carboxylic acid ethyl ester 867187-86-8P, 6-Methyl-1-oxo-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867187-87-9P, 6-Bromomethyl-1-oxo-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867187-88-0P, 6-[(Morpholin-4-yl)methyl]-1-oxo-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867187-90-4P, 1-Oxo-3-phenyl-6-(3-phenylpropoxy)-1H-indene-2-carboxylic acid methyl ester 867214-90-2P, 6-Methoxy-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867214-92-4P, 2-(3-Methoxybenzyl)-3-oxo-3-phenylpropionic acid ethyl ester 867215-03-0P, 6-[2-(Pyridin-2-yl)ethoxy]-1-oxo-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867215-05-2P, 3-Phenyl-6-(3-phenylpropoxy)inden-1-one 867215-06-3P, 2-Bromo-3-phenyl-6-(3-phenylpropoxy)inden-1-one 867215-14-3P, 1-Bromo-6-methoxy-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867215-17-6P, 1-Hydroxyimino-6-methoxy-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867215-20-1P, 6-Hydroxy-1-oxo-3-phenyl-1H-indene-2-carboxylic acid methyl ester 867215-21-2P, 6-Hydroxy-1-oxo-3-phenyl-1H-indene-2-carboxylic acid 867215-22-3P, 6-Hydroxy-1-oxo-3-phenyl-1H-indene-2-carboxylic acid cyclohexylamide 867215-23-4P, 6-[2-(Morpholin-4-yl)ethoxy]-1-oxo-3-phenyl-1H-indene-2-carboxylic acid cyclohexylamide 867215-24-5P, 1-Hydroxyimino-6-[2-(morpholin-4-yl)ethoxy]-3-phenyl-1H-indene-2-carboxylic acid cyclohexylamide 867215-26-7P, 1-Hydroxyimino-3-phenyl-6-(3-phenylpropoxy)-1H-indene-2-carbonitrile
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of indenes as selective modulators of peroxisome proliferator activated receptors)

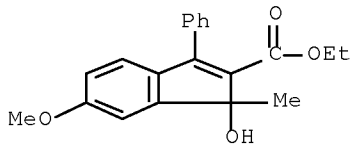
IT 50-99-7, D-Glucose, biological studies
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(reducers of blood glucose levels; preparation of indenes as selective modulators of peroxisome proliferator activated receptors)

IT 867214-93-5P, 1-Hydroxy-6-methoxy-1,3-diphenyl-1H-indene-2-carboxylic acid ethyl ester 867214-96-8P, 1-Hydroxy-6-methoxy-1-methyl-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867214-97-9P, 1-Benzyl-1-hydroxy-6-methoxy-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867214-98-0P, 1-Cyclohexyl-1-hydroxy-6-methoxy-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867214-99-1P, 1-Hydroxy-1,3-diphenyl-6-(3-phenylpropoxy)-1H-indene-2-carboxylic acid ethyl ester 867215-16-5P, 1-Amino-6-methoxy-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867215-18-7P, 1-Amino-3-phenyl-6-(3-phenylpropoxy)-1H-indene-2-carboxylic acid ethyl ester 867215-19-8P, 1-Amino-6-[2-(morpholin-4-yl)ethoxy]-3-phenyl-1H-indene-2-carboxylic acid cyclohexylamide
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(drug candidate; preparation of indenes as selective modulators of peroxisome proliferator activated receptors)

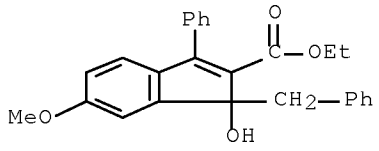
RN 867214-93-5 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-hydroxy-6-methoxy-1,3-diphenyl-, ethyl ester (CA INDEX NAME)



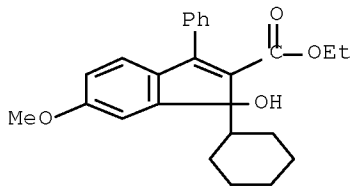
RN 867214-96-8 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-hydroxy-6-methoxy-1-methyl-3-phenyl-, ethyl ester (CA INDEX NAME)



RN 867214-97-9 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-hydroxy-6-methoxy-3-phenyl-1-(phenylmethyl)-, ethyl ester (CA INDEX NAME)

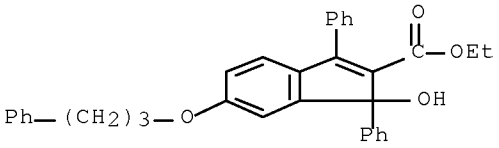


RN 867214-98-0 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-cyclohexyl-1-hydroxy-6-methoxy-3-phenyl-, ethyl ester (CA INDEX NAME)



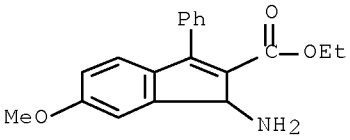
RN 867214-99-1 ZCAPLUS

CN 1H-Indene-2-carboxylic acid, 1-hydroxy-1,3-diphenyl-6-(3-phenylpropoxy)-, ethyl ester (CA INDEX NAME)



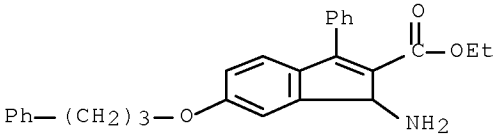
RN 867215-16-5 ZCAPLUS

CN 1H-Indene-2-carboxylic acid, 1-amino-6-methoxy-3-phenyl-, ethyl ester (CA INDEX NAME)



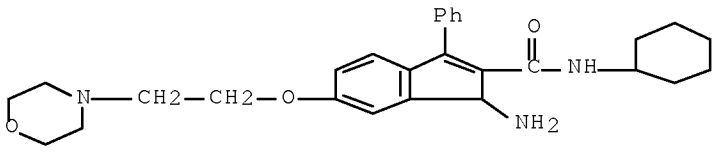
RN 867215-18-7 ZCAPLUS

CN 1H-Indene-2-carboxylic acid, 1-amino-3-phenyl-6-(3-phenylpropoxy)-, ethyl ester (CA INDEX NAME)



RN 867215-19-8 ZCAPLUS

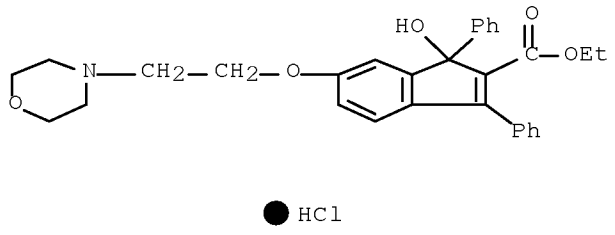
CN 1H-Indene-2-carboxamide, 1-amino-N-cyclohexyl-6-[2-(4-morpholinyl)ethoxy]-3-phenyl- (CA INDEX NAME)



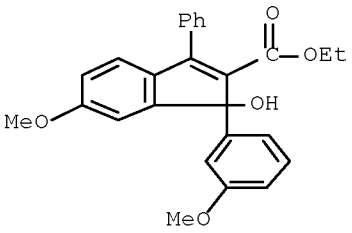
IT 867187-97-1P, 1-Hydroxy-6-[2-(morpholin-4-yl)ethoxy]-1,3-diphenyl-1H-indene-2-carboxylic acid ethyl ester hydrochloride 867214-94-6P , 1-Hydroxy-6-methoxy-1-(3-methoxyphenyl)-3-phenyl-1H-indene-2-carboxylic

acid ethyl ester 867214-95-7P, 1-Hydroxy-1-isopropyl-6-methoxy-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867215-00-7P, 1-Hydroxy-6-[2-(morpholin-4-yl)ethoxy]-1,3-diphenyl-1H-indene-2-carboxylic acid ethyl ester 867215-01-8P, 1-Hydroxy-6-[(morpholin-4-yl)methyl]-1,3-diphenyl-1H-indene-2-carboxylic acid ethyl ester 867215-02-9P, 1-Hydroxy-1,3-diphenyl-6-[2-(pyridin-2-yl)ethoxy]-1H-indene-2-carboxylic acid ethyl ester 867215-04-1P, 1-Hydroxy-1,3-diphenyl-6-(3-phenylpropoxy)-1H-indene-2-carbonitrile 867215-07-4P, 1-Hydroxy-1,3-diphenyl-6-(3-phenylpropoxy)-1H-indene-2-carboxylic acid methyl ester 867215-08-5P, 1-Hydroxy-6-methoxy-1,3-diphenyl-1H-indene-2-carboxylic acid 867215-09-6P, 1-Hydroxy-6-methoxy-1-methyl-3-phenyl-1H-indene-2-carboxylic acid 867215-10-9P, 1-Benzyl-1-hydroxy-6-methoxy-3-phenyl-1H-indene-2-carboxylic acid 867215-11-0P, 1-Hydroxy-1,3-diphenyl-6-(3-phenylpropoxy)-1H-indene-2-carboxylic acid 867215-12-1P, 1-Cyclohexyl-1-hydroxy-6-methoxy-3-phenyl-1H-indene-2-carboxylic acid 867215-13-2P, 1,6-Dimethoxy-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867215-15-4P, 1-Ethoxy-6-methoxy-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867215-25-6P, 1-Amino-3-phenyl-6-(3-phenylpropoxy)-1H-indene-2-carbonitrile 867215-27-8P, 1-Acetylamino-6-methoxy-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867215-28-9P, 6-Methoxy-3-phenyl-1-propionylamino-1H-indene-2-carboxylic acid ethyl ester 867215-29-0P, 1-Acetylamino-3-phenyl-6-(3-phenylpropoxy)-1H-indene-2-carboxylic acid ethyl ester 867215-30-3P, 1-Acetylamino-6-[2-(morpholin-4-yl)ethoxy]-3-phenyl-1H-indene-2-carboxylic acid cyclohexylamide 867215-31-4P, 1-Diethylamino-6-methoxy-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867215-32-5P, 1-Ethylamino-6-methoxy-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867215-33-6P, 6-Methoxy-1-(morpholin-4-yl)-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867215-34-7P, 1-Benzylamino-6-methoxy-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867215-35-8P, 1-Cyclohexylamino-6-methoxy-3-phenyl-1H-indene-2-carboxylic acid ethyl ester
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of indenes as selective modulators of peroxisome proliferator activated receptors)

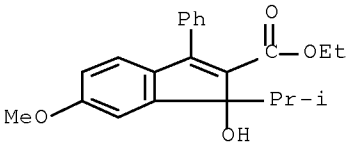
RN 867187-97-1 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-hydroxy-6-[2-(4-morpholinyl)ethoxy]-1,3-diphenyl-, ethyl ester, hydrochloride (1:1) (CA INDEX NAME)



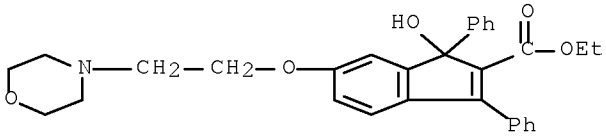
RN 867214-94-6 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-hydroxy-6-methoxy-1-(3-methoxyphenyl)-3-phenyl-, ethyl ester (CA INDEX NAME)



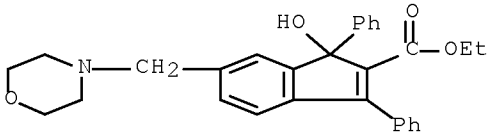
RN 867214-95-7 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-hydroxy-6-methoxy-1-(1-methylethyl)-3-phenyl-, ethyl ester (CA INDEX NAME)



RN 867215-00-7 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-hydroxy-6-[2-(4-morpholinyl)ethoxy]-1,3-diphenyl-, ethyl ester (CA INDEX NAME)

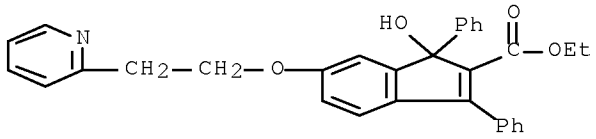


RN 867215-01-8 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-hydroxy-6-(4-morpholinylmethyl)-1,3-diphenyl-, ethyl ester (CA INDEX NAME)

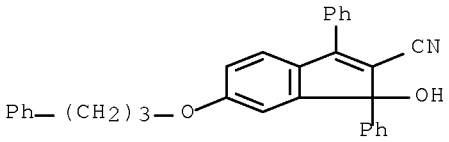


RN 867215-02-9 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-hydroxy-1,3-diphenyl-6-[2-(2-

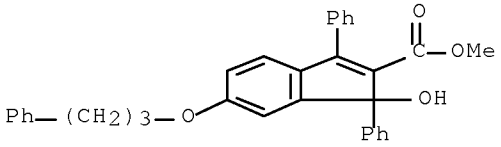
pyridinyl)ethoxy]-, ethyl ester (CA INDEX NAME)



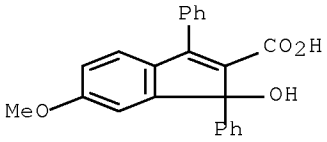
RN 867215-04-1 ZCAPLUS
CN 1H-Indene-2-carbonitrile, 1-hydroxy-1,3-diphenyl-6-(3-phenylpropoxy)- (CA INDEX NAME)



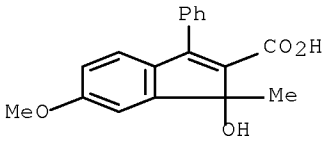
RN 867215-07-4 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-hydroxy-1,3-diphenyl-6-(3-phenylpropoxy)-, methyl ester (CA INDEX NAME)



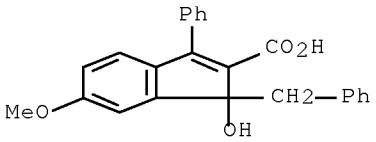
RN 867215-08-5 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-hydroxy-6-methoxy-1,3-diphenyl- (CA INDEX NAME)



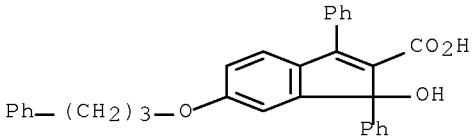
RN 867215-09-6 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-hydroxy-6-methoxy-1-methyl-3-phenyl- (CA INDEX NAME)



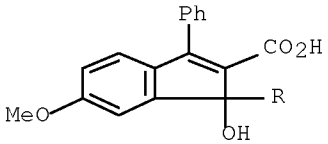
RN 867215-10-9 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-hydroxy-6-methoxy-3-phenyl-1-(phenylmethyl)-
(CA INDEX NAME)

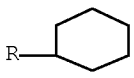


RN 867215-11-0 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-hydroxy-1,3-diphenyl-6-(3-phenylpropoxy)-
(CA INDEX NAME)



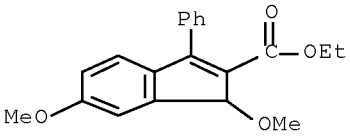
RN 867215-12-1 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-cyclohexyl-1-hydroxy-6-methoxy-3-phenyl-
(CA INDEX NAME)



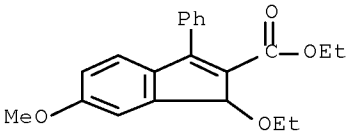


RN 867215-13-2 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1,6-dimethoxy-3-phenyl-, ethyl ester (CA

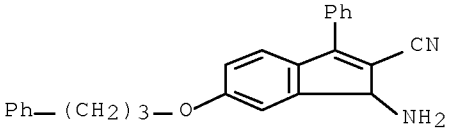
INDEX NAME)



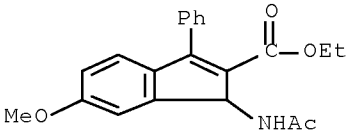
RN 867215-15-4 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-ethoxy-6-methoxy-3-phenyl-, ethyl ester (CA INDEX NAME)



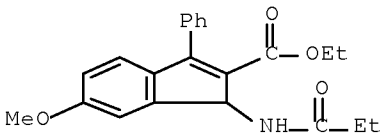
RN 867215-25-6 ZCAPLUS
CN 1H-Indene-2-carbonitrile, 1-amino-3-phenyl-6-(3-phenylpropoxy)- (CA INDEX NAME)



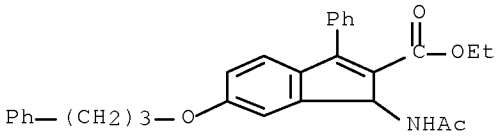
RN 867215-27-8 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-(acetylamino)-6-methoxy-3-phenyl-, ethyl ester (CA INDEX NAME)



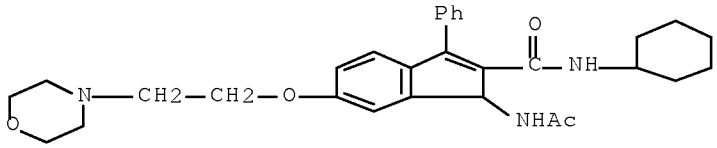
RN 867215-28-9 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 6-methoxy-1-[(1-oxopropyl)amino]-3-phenyl-, ethyl ester (CA INDEX NAME)



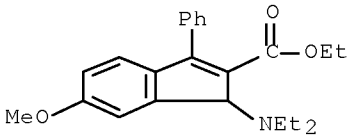
RN 867215-29-0 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-(acetylamino)-3-phenyl-6-(3-phenylpropoxy)-, ethyl ester (CA INDEX NAME)



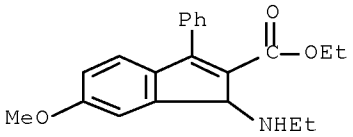
RN 867215-30-3 ZCAPLUS
CN 1H-Indene-2-carboxamide, 1-(acetylamino)-N-cyclohexyl-6-[2-(4-morpholinyl)ethoxy]-3-phenyl- (CA INDEX NAME)



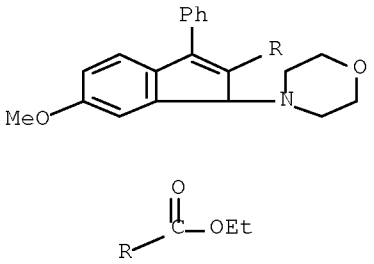
RN 867215-31-4 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-(diethylamino)-6-methoxy-3-phenyl-, ethyl ester (CA INDEX NAME)



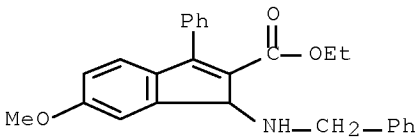
RN 867215-32-5 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-(ethylamino)-6-methoxy-3-phenyl-, ethyl ester (CA INDEX NAME)



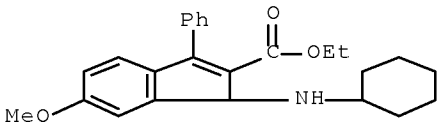
RN 867215-33-6 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 6-methoxy-1-(4-morpholinyl)-3-phenyl-, ethyl ester (CA INDEX NAME)



RN 867215-34-7 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 6-methoxy-3-phenyl-1-[(phenylmethyl)amino]-, ethyl ester (CA INDEX NAME)



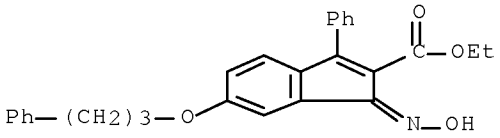
RN 867215-35-8 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-(cyclohexylamino)-6-methoxy-3-phenyl-, ethyl ester (CA INDEX NAME)



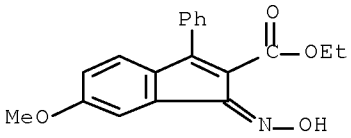
IT 867187-60-8P, 1-Hydroxyimino-3-phenyl-6-(3-phenylpropoxy)-1H-indene-2-carboxylic acid ethyl ester 867215-17-6P, 1-Hydroxyimino-6-methoxy-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867215-24-5P, 1-Hydroxyimino-6-[2-(morpholin-4-yl)ethoxy]-3-phenyl-

1H-indene-2-carboxylic acid cyclohexylamide 867215-26-7P, 1-Hydroxyimino-3-phenyl-6-(3-phenylpropoxy)-1H-indene-2-carbonitrile
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of indenes as selective modulators of peroxisome proliferator activated receptors)

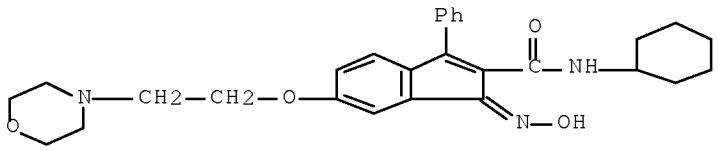
RN 867187-60-8 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-(hydroxyimino)-3-phenyl-6-(3-phenylpropoxy)-, ethyl ester (CA INDEX NAME)



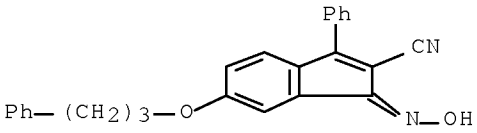
RN 867215-17-6 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-(hydroxyimino)-6-methoxy-3-phenyl-, ethyl ester (CA INDEX NAME)



RN 867215-24-5 ZCAPLUS
CN 1H-Indene-2-carboxamide, N-cyclohexyl-1-(hydroxyimino)-6-[2-(4-morpholinyl)ethoxy]-3-phenyl- (CA INDEX NAME)



RN 867215-26-7 ZCAPLUS
CN 1H-Indene-2-carbonitrile, 1-(hydroxyimino)-3-phenyl-6-(3-phenylpropoxy)- (CA INDEX NAME)



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

```
=> file registry
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DICTIONARY FILE UPDATES:  22 JUN 2008  HIGHEST RN 1029806-10-7

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TSCA INFORMATION NOW CURRENT THROUGH January 9, 2008.

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
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experimental property data in the original document.  For information
on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

Uploading L5.str
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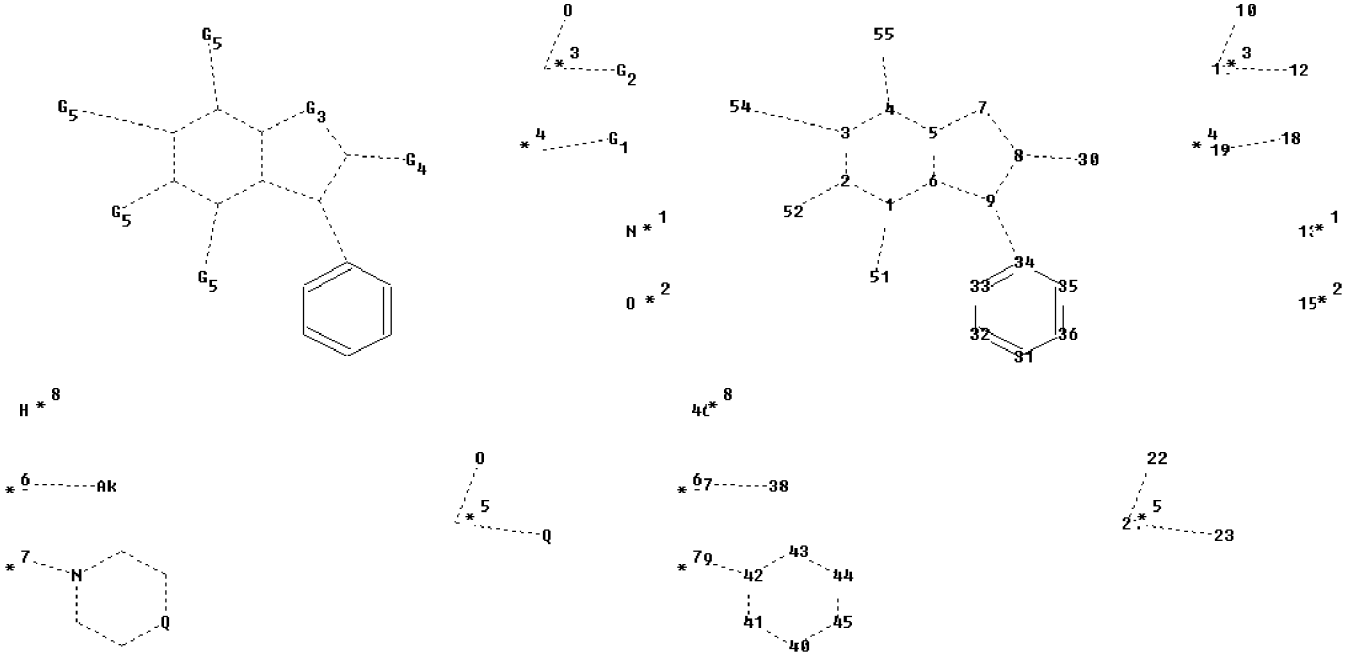

```
chain nodes :
10  12  15  18  21  22  23  30  37  38  39  46  51  52  54  55
ring nodes :
1  2  3  4  5  6  7  8  9  11  19  31  32  33  34  35  36  40  41  42  43  44  45

ring/chain nodes :
13
```

```
chain bonds :
1-51  2-52  3-54  4-55  8-30  9-34  10-11  11-12  18-19  21-22  21-23  37-38  39-42

ring bonds :
1-2  1-6  2-3  3-4  4-5  5-6  5-7  6-9  7-8  8-9  31-32  31-36  32-33  33-34  34-35
35-36  40-41  40-45  41-42  42-43  43-44  44-45
exact/norm bonds :
1-2  1-6  1-51  2-3  2-52  3-4  3-54  4-5  4-55  5-6  5-7  6-9  7-8  8-9  8-30  9-
34
10-11  11-12  18-19  21-22  21-23  37-38  39-42  40-41  40-45  41-42  42-43  43-44
44-45
normalized bonds :
31-32  31-36  32-33  33-34  34-35  35-36


G1:[*1],[*2]

G2:Cb,Ak

G3:[*3],[*4]

G4:CN,[*5]

G5:[*6],[*7],[*8]

Connectivity :
21:3 E exact RC ring/chain  22:1 E exact RC ring/chain
Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  7:Atom  8:Atom  9:Atom  10:CLASS
11:Atom  12:CLASS  13:CLASS  15:CLASS  18:CLASS  19:Atom  21:CLASS  22:CLASS
23:CLASS  30:CLASS
31:Atom  32:Atom  33:Atom  34:Atom  35:Atom  36:Atom  37:CLASS  38:CLASS  39:CLASS
40:Atom  41:Atom
42:Atom  43:Atom  44:Atom  45:Atom  46:CLASS  51:CLASS  52:CLASS  54:CLASS
55:CLASS



Uploading L25.str
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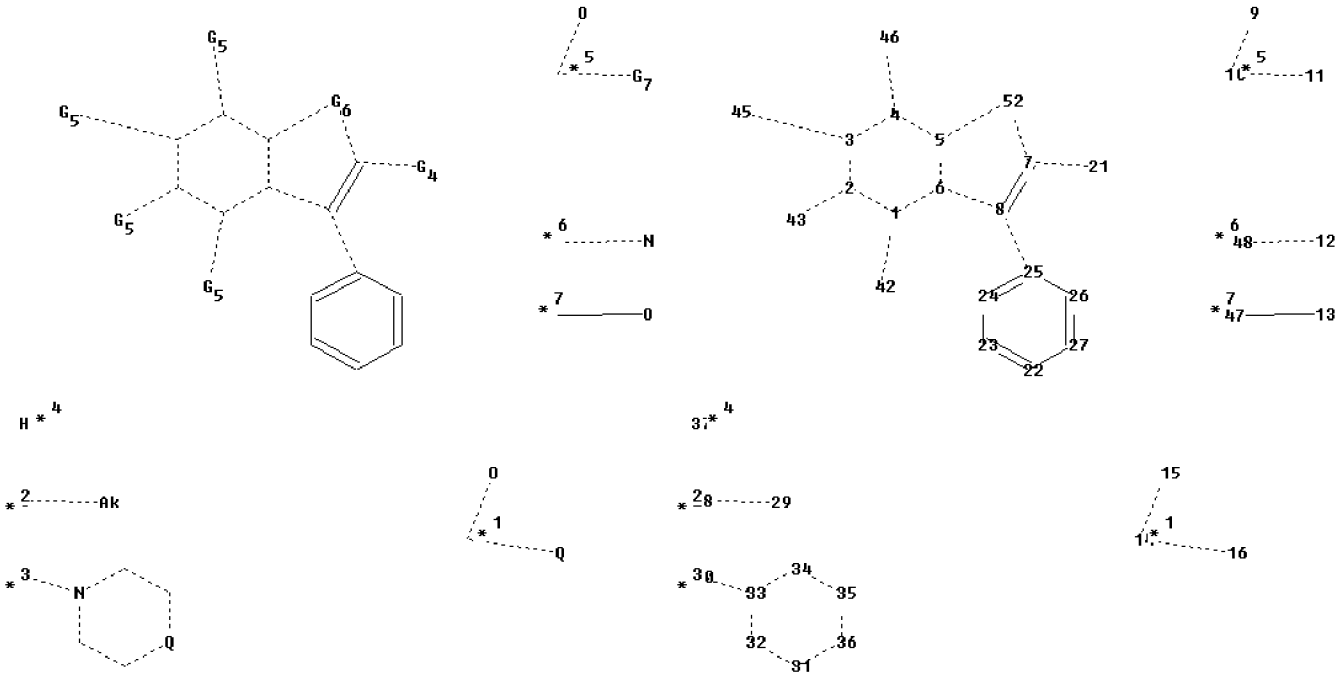


chain nodes :
9 11 13 14 15 16 21 28 29 30 37 42 43 45 46
ring nodes :
1 2 3 4 5 6 7 8 10 22 23 24 25 26 27 31 32 33 34 35 36 47 48 52
ring/chain nodes :
12
chain bonds :
1-42 2-43 3-45 4-46 7-21 8-25 9-10 10-11 12-48 13-47 14-15 14-16 28-29 30-33
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-52 6-8 7-8 7-52 22-23 22-27 23-24 24-25 25-26
26-27 31-32 31-36 32-33 33-34 34-35 35-36
exact/norm bonds :
1-2 1-6 1-42 2-3 2-43 3-4 3-45 4-5 4-46 5-6 5-52 6-8 7-21 7-8 7-52 8-25 9-10 10-11 12-48 13-47 14-15 14-16 28-29 30-33 31-32 31-36 32-33 33-34 34-35 35-36

normalized bonds :
22-23 22-27 23-24 24-25 25-26 26-27

G4:CN,[*1]

G5:[*2],[*3],[*4]

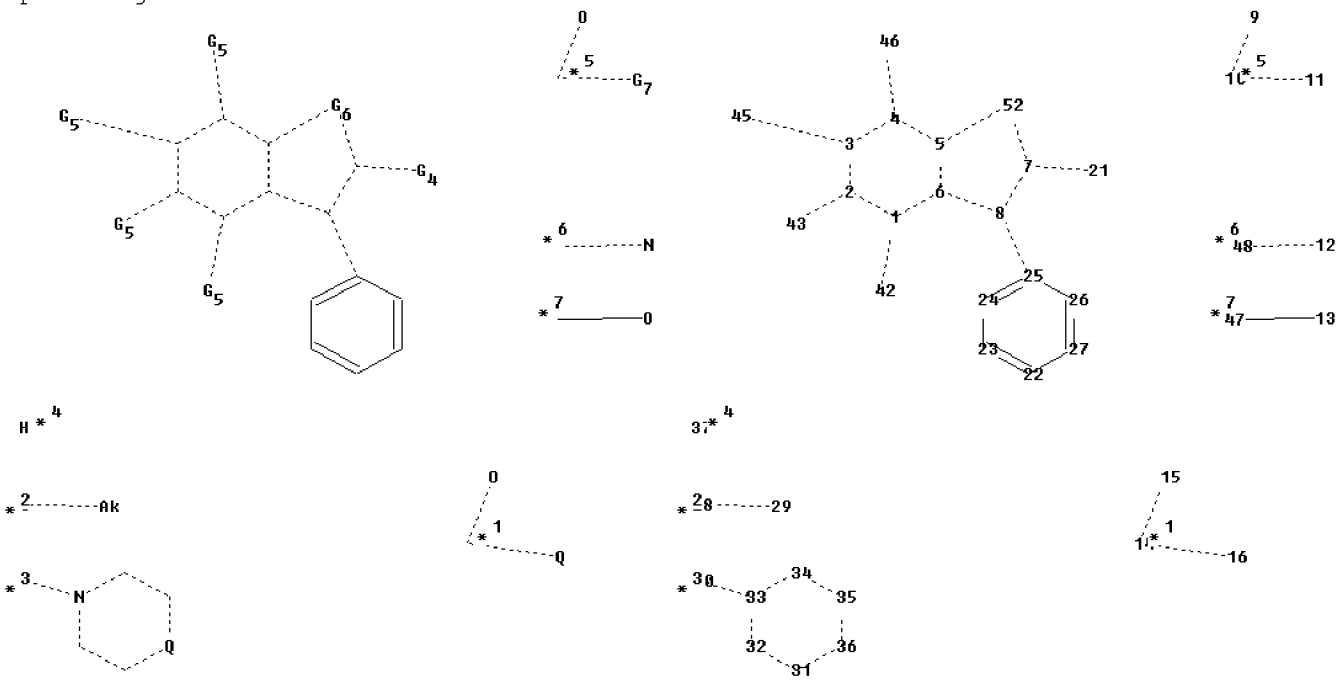
G6:[*5],[*6],[*7]

G7:Cb,Ak

Connectivity :
14:3 E exact RC ring/chain 15:1 E exact RC ring/chain
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:CLASS 10:Atom 11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 21:CLASS 22:Atom

23:Atom 24:Atom 25:Atom
26:Atom 27:Atom 28:CLASS 29:CLASS 30:CLASS 31:Atom 32:Atom 33:Atom 34:Atom
35:Atom
36:Atom 37:CLASS 42:CLASS 43:CLASS 45:CLASS 46:CLASS 47:CLASS 48:CLASS
52:CLASS

Uploading L37.str



chain nodes :
9 11 13 14 15 16 21 28 29 30 37 42 43 45 46
ring nodes :
1 2 3 4 5 6 7 8 10 22 23 24 25 26 27 31 32 33 34 35 36 47 48
52
ring/chain nodes :
12
chain bonds :
1-42 2-43 3-45 4-46 7-21 8-25 9-10 10-11 12-48 13-47 14-15 14-16 28-29
30-33
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-52 6-8 7-8 7-52 22-23 22-27 23-24 24-25 25-
26
26-27 31-32 31-36 32-33 33-34 34-35 35-36
exact/norm bonds :
1-2 1-6 1-42 2-3 2-43 3-4 3-45 4-5 4-46 5-6 5-52 6-8 7-21 7-8 7-52
8-25 9-10 10-11 12-48 13-47 14-15 14-16 28-29 30-33 31-32 31-36 32-33
33-34 34-35 35-36

normalized bonds :
22-23 22-27 23-24 24-25 25-26 26-27

G4:CN,[*1]

G5:[*2],[*3],[*4]

```
G6:[*5],[*6],[*7]

G7:Cb,Ak

Connectivity :
7:3 E exact RC ring/chain  8:3 E exact RC ring/chain  14:3 E exact RC ring/chain
15:1 E exact RC ring/chain  47:3 E exact RC ring/chain  48:3 E exact RC ring/chain
Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  7:Atom  8:Atom  9:CLASS  10:Atom
11:CLASS  12:CLASS  13:CLASS  14:CLASS  15:CLASS  16:CLASS  21:CLASS  22:Atom
23:Atom  24:Atom  25:Atom
26:Atom  27:Atom  28:CLASS  29:CLASS  30:CLASS  31:Atom  32:Atom  33:Atom  34:Atom
35:Atom
36:Atom  37:CLASS  42:CLASS  43:CLASS  45:CLASS  46:CLASS  47:CLASS  48:CLASS
52:CLASS




=> file zcaplus
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FILE LAST UPDATED: 22 Jun 2008  (20080622/ED)

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  This file contains CAS Registry Numbers for easy and accurate
  substance identification.
'OBI' IS DEFAULT SEARCH FIELD FOR 'ZCAPLUS' FILE

=> d stat que L28
L5              STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -  AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.
L7          427 SEA FILE=REGISTRY SSS FUL L5
L25             STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -  AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.
L27         166 SEA FILE=REGISTRY SUB=L7 SSS FUL L25
L28          35 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  L27
```

```
=> d stat que L42
L5              STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -  AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.
L7          427 SEA FILE=REGISTRY SSS FUL L5
L37             STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -  AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.
L40         196 SEA FILE=REGISTRY SUB=L7 SSS FUL L37
L42          47 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  L40


=> d stat que L81
L5              STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -  AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.
L7          427 SEA FILE=REGISTRY SSS FUL L5
L25             STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -  AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.
L27         166 SEA FILE=REGISTRY SUB=L7 SSS FUL L25
L28          35 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  L27
L37             STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -  AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.
L40         196 SEA FILE=REGISTRY SUB=L7 SSS FUL L37
L42          47 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  L40
L54      171149 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  ?DIABET?/BI
L55       56841 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  OBES?/BI
L56       11261 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  ANTIOBES?/BI
L57      289180 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  ?ARTER?/BI
L58      504356 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  ?LIPID?/BI
L59      225556 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  ?INSULIN?/BI
L60      124786 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  ?HYPERTENS?/BI
L61       32726 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  ?HYPOTENS?/BI
L62       89940 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  ?OSTEO?/BI
L63      594903 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  LIVER/BI
L64       25633 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  ?CIRRHOS?/BI
L65       45105 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  ?ASTHMA?/BI
L66      553816 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  ?NEOPLAS?/BI
L67      407468 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  ?CANCER?/BI
L68      662469 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  ?TUMOR?/BI
L69        5585 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  ?TUMOUR?/BI
L70       56405 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  ?SARCOMA?/BI
L71      123066 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  ?LEUKEM?/BI
L72        1597 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  ?LEUKAEM?/BI
L73      308147 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  ?CARCINO?/BI
L74       44793 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  ?LYMPHOM?/BI
L75       39743 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  ?MELANOM?/BI
```

```
L76       51481 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  ?ANGIOGEN?/BI
L78       11482 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  PPAR/BI
L79       23760 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  PEROXISOM?/BI
L81          12 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  (L28 OR L42) AND (L54 OR L55
                 OR L56 OR L57 OR L58 OR L59 OR L60 OR L61 OR L62 OR L63 OR L64
                 OR L65 OR L66 OR L67 OR L68 OR L69 OR L70 OR L71 OR L72 OR L73
                 OR L74 OR L75 OR L76 OR L78 OR L79)


=> s (L28 or L42 or L81) not L102,L101
L103        40 (L28 OR L42 OR L81) NOT (L102 OR L101)

=> s L103 and (L47,L82)
L104        14 L103 AND ((L47 OR L82))

=> s L103 or L014
             0 L014/OBI
L105        40 L103 OR L014/OBI

=> s L103 or L104
L106        40 L103 OR L104

=> d ibib abs hitind hitstr L106 1-40

L106 ANSWER 1 OF 40  ZCAPLUS  COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER:        2008:330295  ZCAPLUS  Full-text
DOCUMENT NUMBER:         148:332089
TITLE:                   Anionic Polymerization of a Benzofulvene Monomer
                         Leading to a Thermoreversible π-Stacked Polymer.
                         Studies in Macromolecular and Aggregate Structure
AUTHOR(S):               Cappelli, Andrea; Galeazzi, Simone; Giuliani, Germano;
                         Anzini, Maurizio; Aggravi, Marianna; Donati,
                         Alessandro; Zetta, Lucia; Boccia, Antonella Caterina;
                         Mendichi, Raniero; Giorgi, Gianluca; Paccagnini,
                         Eugenio; Vomero, Salvatore
CORPORATE SOURCE:        Dipartimento Farmaco Chimico Tecnologico and European
                         Research Centre for Drug Discovery and Development,
                         Universita degli Studi di Siena, Siena, 53100, Italy
SOURCE:                  Macromolecules (Washington, DC, United States) (2008),
                         41(7), 2324-2334
                         CODEN: MAMOBX; ISSN: 0024-9297
PUBLISHER:               American Chemical Society
DOCUMENT TYPE:           Journal
LANGUAGE:                English
AB    The polymerization of trans-diene BF1 [ethyl 1-methylene-3-(4-methylphenyl)-
      1H- indene-2-carboxylate] was studied in the presence of various amts. of an
      anionic initiator such as phenyllithium to obtain information on the
      properties of this diene monomer and on its polymers.  The anionic
      polymerization of BF1 produced a mixture of oligomers and a polymer (poly-BF1-
      AP), the proportion of which is regulated by the amount of the initiator used.
      Poly-BF1 was separated from lower oligomers on the basis of the solubility in
      n-hexane, and the soluble material was further fractionated by chromatog. to
      obtain activated monomers and dimers.  The structure of dimers and poly-BF1-AP
      was studied by NMR spectroscopy, absorption and emission spectroscopy, and
      mass spectrometry.  The whole set of results is consistent, confirming for
      poly-BF1 a vinyl (1,2) polymer chaining stabilized by aromatic stacking
      interactions.  The thermoreversibility of poly-BF1-AP was characterized by 1H
      NMR and compared to its DSC features. Remarkably, SEC-MALS anal. showed that
      the mol. weight of poly-BF1-AP is relatively low (about 10 kg/mol), and SEM
      studies revealed that the polymer is liable to give nanospheres and
```

microspheres showing favorable shapes and dimensions. These results suggest the potential tuning of the material properties of these π-stacked polymers by the regulation of the mol. weight

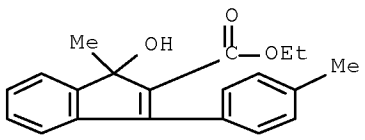
CC 35-4 (Chemistry of Synthetic High Polymers)

IT 637760-42-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(in thesis of thermoreversible oligomers and polymers from benzofulvene derivative via anionic polymerization)

IT 637760-42-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(in thesis of thermoreversible oligomers and polymers from benzofulvene derivative via anionic polymerization)

RN 637760-42-0 ZCAPLUS

CN 1H-Indene-2-carboxylic acid, 1-hydroxy-1-methyl-3-(4-methylphenyl)-, ethyl ester (CA INDEX NAME)



REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L106 ANSWER 2 OF 40 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2007:1258606 ZCAPLUS Full-text

DOCUMENT NUMBER: 148:100367

TITLE: Cationic Palladium(II)-Catalyzed Highly Enantioselective [3 + 2] Annulation of 2-Acylarylboronic Acids with Substituted Alkynes

AUTHOR(S): Yang, Miao; Zhang, Xumu; Lu, Xiyan

CORPORATE SOURCE: State Key Laboratory of Organometallic Chemistry, Shanghai Institute of Organic Chemistry, Chinese Academy of Science, Shanghai, 200032, Peop. Rep. China

SOURCE: Organic Letters (2007), 9(24), 5131-5133
CODEN: ORLEF7; ISSN: 1523-7060

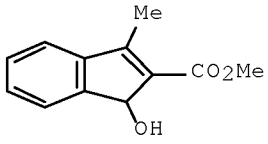
PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 148:100367

GI



I

AB A cationic palladium(II)-catalyzed enantioselective tandem [3 + 2] annulation of 2-acylarylboronic acids with substituted alkynes employing chiral biarylphosphine ligand to yield optically active 1-indenols, e.g., I, was developed in high yields and excellent enantioselectivities.

CC 25-23 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)

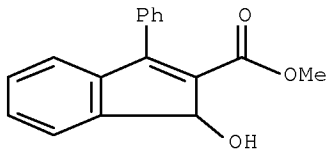
IT 1000204-52-3P 1000204-53-4P 1000204-54-5P 1000204-55-6P
1000204-56-7P 1000204-57-8P 1000204-58-9P
1000204-59-0P 1000204-60-3P 1000204-61-4P 1000204-62-5P
1000204-63-6P 1000204-64-7P 1000204-65-8P 1000204-67-0P
1000204-69-2P 1000204-70-5P 1000204-71-6P 1000204-72-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(stereoselective preparation of indenols via cationic palladium-catalyzed enantioselective [3+2] annulation of acylarylboronic acids/esters with alkynes in presence of chiral biarylphosphine ligand)

IT 1000204-56-7P 1000204-57-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(stereoselective preparation of indenols via cationic palladium-catalyzed enantioselective [3+2] annulation of acylarylboronic acids/esters with alkynes in presence of chiral biarylphosphine ligand)

RN 1000204-56-7 ZCAPLUS

CN 1H-Indene-2-carboxylic acid, 1-hydroxy-3-phenyl-, methyl ester, (+)- (CA INDEX NAME)

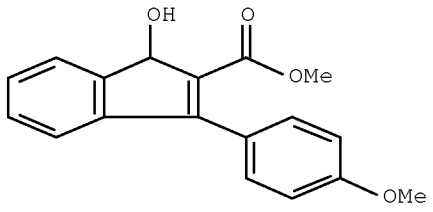
Rotation (+).



RN 1000204-57-8 ZCAPLUS

CN 1H-Indene-2-carboxylic acid, 1-hydroxy-3-(4-methoxyphenyl)-, methyl ester, (+)- (CA INDEX NAME)

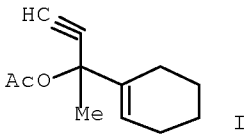
Rotation (+).



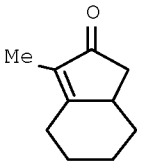
REFERENCE COUNT: 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L106 ANSWER 3 OF 40 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2007:1050869 ZCAPLUS Full-text
DOCUMENT NUMBER: 147:521894
TITLE: Palladium(II)- and mercury(II)-catalyzed rearrangements of propargyl acetates

AUTHOR(S): Caruana, Patrick A.; Frontier, Alison J.
CORPORATE SOURCE: Department of Chemistry, University of Rochester, Rochester, NY, 14627, USA
SOURCE: Tetrahedron (2007), 63(43), 10646-10656
CODEN: TETRAB; ISSN: 0040-4020
PUBLISHER: Elsevier Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 147:521894
GI

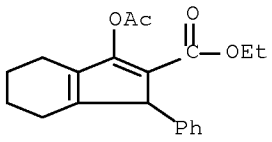


I



II

AB The scope and utility of the metal-catalyzed rearrangement of propargyl acetates first reported by Rautenstrauch were expanded. Treatment of a series of appropriate acetate substrates with Pd(II)- and Hg(II)-catalysts afforded synthetically useful fused 5,6-bicyclic-1,4-cyclopentadienyl acetates and 2-cyclopentenones. E.g., PdCl2-catalyzed rearrangement of propargyl acetate I gave 56% 2-cyclopentenone derivative II. It was found that the substituents at the terminal alkynyl and alkenyl positions of the acetate substrate had a significant impact on the outcome of the reaction.
CC 24-7 (Alicyclic Compounds)
IT 24730-98-1P 88364-52-7P 881688-53-5P 956584-61-5P
956584-62-6P 956584-63-7P 956584-64-8P 956584-70-6P
956584-71-7P 956584-72-8P 956584-73-9P 956584-74-0P 956584-75-1P
956584-77-3P 956584-78-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and palladium(II)- and mercury(II)-catalyzed rearrangements of propargyl acetates)
IT 956584-62-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and palladium(II)- and mercury(II)-catalyzed rearrangements of propargyl acetates)
RN 956584-62-6 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 3-(acetyloxy)-4,5,6,7-tetrahydro-1-phenyl-, ethyl ester (CA INDEX NAME)



REFERENCE COUNT: 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L106 ANSWER 4 OF 40 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2007:355089 ZCAPLUS Full-text
DOCUMENT NUMBER: 146:522144
TITLE: Structural Manipulation of Benzofulvene Derivatives Showing Spontaneous Thermoreversible Polymerization. Role of the Substituents in the Modulation of Polymer Properties
AUTHOR(S): Cappelli, Andrea; Galeazzi, Simone; Giuliani, Germano; Anzini, Maurizio; Donati, Alessandro; Zetta, Lucia; Mendichi, Raniero; Aggravi, Marianna; Giorgi, Gianluca; Paccagnini, Eugenio; Vomero, Salvatore
CORPORATE SOURCE: Dipartimento Farmaco Chimico Tecnologico and European Research Centre for Drug Discovery and Development, Universita degli Studi di Siena, Siena, 53100, Italy
SOURCE: Macromolecules (Washington, DC, United States) (2007), 40(9), 3005-3014
CODEN: MAMOBX; ISSN: 0024-9297
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The synthesis of a series of benzofulvene derivs. 3 related to the recently studied Et 1-methylene-3-(4-methylphenyl)-1H-indene-2-carboxylate (BF1) is described. The properties of these trans-diene derivs. were characterized with regard to their capability of polymerizing spontaneously to give new polymers based on functionalized indene monomeric units. The series of polymers has been investigated by NMR spectroscopy, multiangle light scattering online to size exclusion chromatog., UV-vis spectroscopy, mass spectrometry, differential scanning calorimetry, and SEM. The new polymers show very interesting properties such as a thermoreversible polymerization/depolymn., a variable degree of π-stacking, a tendency to give nanostructured macromol. aggregates, and a high solubility in the most common organic solvents. Remarkably, this study demonstrated that most of the polymer properties (e.g. formation, mol. weight, structure, thermoreversibility, and aggregation in nanostructured entities) may be modulated by the stereoelectronic characteristics of the substituents present on the indene moiety.

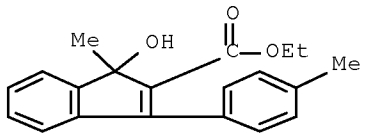
CC 35-4 (Chemistry of Synthetic High Polymers)
Section cross-reference(s): 36

IT 13093-22-6P, 2-Chloro-3-phenyl-1H-1-indenone 13304-52-4P, 2-Methyl-3-phenyl-1H-1-indenone 19772-61-3P 35491-56-6P, 1-Oxo-3-phenyl-1H-2-indenecarbonitrile 94224-67-6P, Ethyl 1-oxo-3-phenyl-1H-2-indenecarboxylate 150192-42-0P, 2-(tert-Butyl)-3-phenyl-1H-1-indenone 150192-43-1P, 3-Phenyl-2-(trimethylsilyl)-1H-1-indenone 222041-22-7P, 1,2-Dimethyl-3-phenyl-1H-1-indenol 637760-42-0P, Ethyl 1-hydroxy-1-methyl-3-(4-methylphenyl)-1H-indene-2-carboxylate 696661-22-0P, 3-(4-Methylphenyl)-1-oxa-1H-2-indenecarbonitrile 696661-26-4P 724776-29-8P, Ethyl 1-hydroxy-1-methyl-3-phenyl-1H-indene-2-carboxylate 937079-92-0P, Ethyl (E)-2-cyano-3-(4-methylphenyl)-3-phenyl-2-propenoate 937079-93-1P, Ethyl (Z)-2-cyano-3-(4-methylphenyl)-3-phenyl-2-propenoate 937079-95-3P, (E)-2-Cyano-3-(4-methylphenyl)-3-phenyl-2-propenoic acid 937079-96-4P, (Z)-2-Cyano-3-(4-methylphenyl)-3-phenyl-2-propenoic acid 937079-97-5P, 6-Methyl-1-oxa-3-phenyl-1H-2-indenecarbonitrile 937079-98-6P, 3-Phenyl-2-[2-(2-pyridyl)-1-ethynyl]-1H-1-indenone 937079-99-7P, N,N-Dimethyl-3-(4-methylphenyl)-1-oxo-1H-2-indenecarboxamide 937080-00-7P, 1-Methyl-3-phenyl-1H-1-indenol 937080-01-8P, 1-Methyl-3-phenyl-2-(trimethylsilyl)-1H-1-indenol 937080-02-9P, 2-Chloro-1-methyl-3-phenyl-1H-1-indenol 937080-04-1P, 2-Bromo-1-methyl-3-phenyl-1H-1-indenol 937080-07-4P,

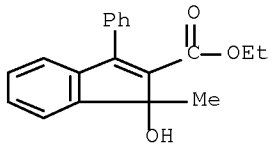
1-Hydroxy-1-methyl-3-phenyl-1H-indene-2-carbonitrile 937080-09-6P
, 1-Hydroxy-1-methyl-3-(4-methylphenyl)-1H-indene-2-carbonitrile
937080-10-9P, 1,6-Dimethyl-1-hydroxy-3-phenyl-1H-indene-2-carbonitrile
937080-11-0P, 1-Methyl-3-phenyl-2-[2-(2-pyridyl)-1-ethynyl]-1H-1-indenol
937080-13-2P, tert-Butyl 1-hydroxy-1-methyl-3-(4-methylphenyl)-1H-
indene-2-carboxylate 937080-15-4P, 1-Hydroxy-3-(4-methylphenyl)-
N,N,1-trimethyl-1H-2-indenecarboxamide 937080-16-5P,
2-(tert-Butyl)-1-methyl-3-phenyl-1H-1-indenol 937080-17-6P,
Ethyl 1-ethyl-1-hydroxy-3-(4-methylphenyl)-1H-indene-2-carboxylate
937080-18-7P, 2-Fluoro-1-methyl-3-phenyl-1H-1-indenol
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(intermediate; preparation of benzofulvene derivs. showing spontaneous
thermoreversible polymerization and role of substituents in modulation of
polymer properties)

IT 637760-42-0P, Ethyl 1-hydroxy-1-methyl-3-(4-methylphenyl)-1H-
indene-2-carboxylate 724776-29-8P, Ethyl 1-hydroxy-1-methyl-3-
phenyl-1H-indene-2-carboxylate 937080-07-4P,
1-Hydroxy-1-methyl-3-phenyl-1H-indene-2-carbonitrile 937080-09-6P
, 1-Hydroxy-1-methyl-3-(4-methylphenyl)-1H-indene-2-carbonitrile
937080-13-2P, tert-Butyl 1-hydroxy-1-methyl-3-(4-methylphenyl)-1H-
indene-2-carboxylate 937080-15-4P, 1-Hydroxy-3-(4-methylphenyl)-
N,N,1-trimethyl-1H-2-indenecarboxamide 937080-17-6P, Ethyl
1-ethyl-1-hydroxy-3-(4-methylphenyl)-1H-indene-2-carboxylate
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(intermediate; preparation of benzofulvene derivs. showing spontaneous
thermoreversible polymerization and role of substituents in modulation of
polymer properties)

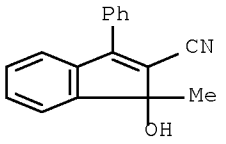
RN 637760-42-0 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-hydroxy-1-methyl-3-(4-methylphenyl)-, ethyl
ester (CA INDEX NAME)



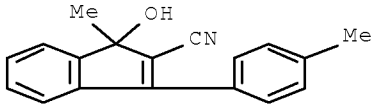
RN 724776-29-8 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-hydroxy-1-methyl-3-phenyl-, ethyl ester
(CA INDEX NAME)



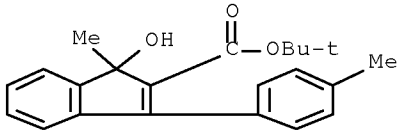
RN 937080-07-4 ZCAPLUS
CN 1H-Indene-2-carbonitrile, 1-hydroxy-1-methyl-3-phenyl- (CA INDEX NAME)



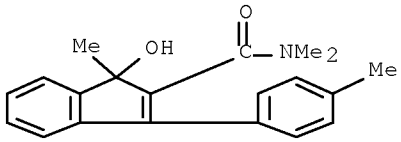
RN 937080-09-6 ZCAPLUS
CN 1H-Indene-2-carbonitrile, 1-hydroxy-1-methyl-3-(4-methylphenyl)- (CA INDEX NAME)



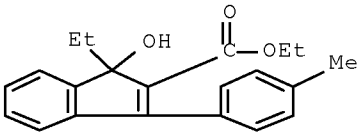
RN 937080-13-2 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-hydroxy-1-methyl-3-(4-methylphenyl)-, 1,1-dimethylethyl ester (CA INDEX NAME)



RN 937080-15-4 ZCAPLUS
CN 1H-Indene-2-carboxamide, 1-hydroxy-N,N,1-trimethyl-3-(4-methylphenyl)- (CA INDEX NAME)



RN 937080-17-6 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-ethyl-1-hydroxy-3-(4-methylphenyl)-, ethyl ester (CA INDEX NAME)

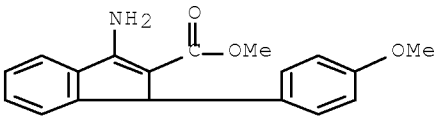


REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L106 ANSWER 5 OF 40 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2007:135659 ZCAPLUS Full-text
DOCUMENT NUMBER: 146:379609
TITLE: Cyclization Reaction of Cyano-Substituted Unsaturated Esters Prompted by Conjugate Addition of Organoborons
AUTHOR(S): Miura, Tomoya; Harumashi, Tatsuro; Murakami, Masahiro
CORPORATE SOURCE: Department of Synthetic Chemistry and Biological Chemistry, Kyoto University, Katsura, Kyoto, 615-8510, Japan
SOURCE: Organic Letters (2007), 9(5), 741-743
CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 146:379609

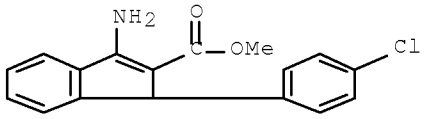
AB Unsatd. esters possessing a pendent cyano moiety react with B-Ar-9-BBNs in the presence of a rhodium(I) catalyst to give five- and six-membered β-enamino esters in good yield. An (oxa-π-allyl)rhodium(I) intermediate, formed by initial conjugate addition of an Ar-rhodium(I) species, undergoes a facile intramol. addition to the cyano group to construct the carbocyclic skeletons.

CC 24-5 (Alicyclic Compounds)
IT 144192-32-5P 932400-33-4P 932400-34-5P 932400-35-6P
932400-36-7P 932400-37-8P 932400-39-0P 932400-42-5P 932400-43-6P
932400-44-7P 932400-45-8P 932400-46-9P 932400-47-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(stereoselective preparation of five- and six-membered β-enamino esters via subsequent conjugate addition and cyclization of unsatd. cycanoesters with B-Ar-9-BBNs catalyzed by rhodium and uses as building blocks.)
IT 932400-33-4P 932400-34-5P 932400-47-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(stereoselective preparation of five- and six-membered β-enamino esters via subsequent conjugate addition and cyclization of unsatd. cycanoesters with B-Ar-9-BBNs catalyzed by rhodium and uses as building blocks.)
RN 932400-33-4 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 3-amino-1-(4-methoxyphenyl)-, methyl ester (CA INDEX NAME)

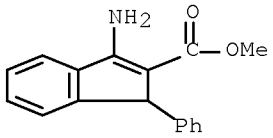


RN 932400-34-5 ZCAPLUS

CN 1H-Indene-2-carboxylic acid, 3-amino-1-(4-chlorophenyl)-, methyl ester (CA INDEX NAME)



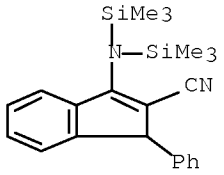
RN 932400-47-0 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 3-amino-1-phenyl-, methyl ester (CA INDEX NAME)



REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L106 ANSWER 6 OF 40 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2007:111693 ZCAPLUS Full-text
DOCUMENT NUMBER: 148:100671
TITLE: Synthesis and crystal structure of 3-(1,1,1,3,3,3-hexamethyl-disilazan-2-yl)-1-phenyl-1H-indene-2-carbonitrile
AUTHOR(S): Liu, Yong-Jun; Zhong, Hua; Qi, Yan; Zhang, Shu-Sheng
CORPORATE SOURCE: College of Chemistry and Molecular Engineering, Qingdao University of Science and Technology, Qingdao, 266042, Peop. Rep. China
SOURCE: Asian Journal of Chemistry (2007), 19(3), 1983-1987
CODEN: AJCHEW; ISSN: 0970-7077
PUBLISHER: Asian Journal of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The crystal structure of 3-(1,1,1,3,3,3-hexamethyl-disilazan-2-yl)-1- phenyl-1H-indene-2-carbonitrile was determined by x-ray diffraction method. The crystal is orthorhombic with space group P212121, a 8.6317(2), b 14.8822(3), c 17.5719(3) Å, I' = 2257.26(8) Å3, Z = 4, and R1 = 0.047, wR2 = 0.129 for 2016 observed reflections (I > 2.00σ(I)). The mean plane of indene is almost perpendicular to the Ph ring attached at chloro atom, the dihedral angling being 84.4(1)°. In the crystal packing, the mols. are stabilized by C-H···π and C-H···N interactions.
CC 29-6 (Organometallic and Organometalloidal Compounds)
Section cross-reference(s): 75
IT 731851-22-2P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(crystal structure; intramol. cyclization and disilylation of dicyanodiphenylethene promoted by samarium /trimethylsilyl chloride to give (hexamethyldisilazanyl)phenylindenecarbonitrile)

IT 731851-22-2P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (crystal structure; intramol. cyclization and disilylation of dicyanodiphenylethene promoted by samarium /trimethylsilyl chloride to give (hexamethyldisilazanyl)phenylindenecarbonitrile)
RN 731851-22-2 ZCAPLUS
CN 1H-Indene-2-carbonitrile, 3-[bis(trimethylsilyl)amino]-1-phenyl- (CA INDEX NAME)



REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L106 ANSWER 7 OF 40 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2006:1045855 ZCAPLUS Full-text
DOCUMENT NUMBER: 145:410050
TITLE: Further Studies on Imidazo[4,5-b]pyridine AT1 Angiotensin II Receptor Antagonists. Effects of the Transformation of the 4-Phenylquinoline Backbone into 4-Phenylisoquinolinone or 1-Phenylindene Scaffolds
AUTHOR(S): Cappelli, Andrea; Mohr, Galla Pericot; Giuliani, Germano; Galeazzi, Simone; Anzini, Maurizio; Mennuni, Laura; Ferrari, Flora; Makovec, Francesco; Kleinrath, Eva M.; Langer, Thierry; Valoti, Massimo; Giorgi, Gianluca; Vomero, Salvatore
CORPORATE SOURCE: Dipartimento Farmaco Chimico Tecnologico and European Research Centre for Drug Discovery and Development, Universita di Siena, Siena, 53100, Italy
SOURCE: Journal of Medicinal Chemistry (2006), 49(22), 6451-6464
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 145:410050

AB The 4-phenylquinoline fragment of novel AT1 receptor antagonists 4 based on imidazo[4,5-b]pyridine moiety was replaced by 4-phenylisoquinolinone (compds. 5) or 1-phenylindene (compds. 6) scaffolds to investigate the structure-activity relationships. Binding studies showed that most of the synthesized compds. display high affinity for the AT1 receptor. Because of the in vitro high potency of carboxylic acids 5b,f, they were evaluated in permeability (in Caco-2 cells) and in pharmacokinetic studies in comparison with quinoline derivs. 4b,i,j,k. The studies showed that these compds. are characterized by rapid excretion, low membrane permeability, and low oral bioavailability. The structure optimization of the indene derivs. led to compds. 6e,f possessing interesting AT1 receptor affinities. Optimization produced polymerizing AT1 receptor ligand 6c, which forms a thermoreversible polymer (poly-6c) and is released from the latter by a temperature-dependent kinetics. The results suggest the possibility of developing novel polymeric prodrugs based on a new

release mechanism. Finally, a set of 34 AT1 receptor antagonists was used as a new test for the evaluation of the predictive capability of the previously published qual. and quant. pharmacophore models.

CC 1-3 (Pharmacology)
Section cross-reference(s): 27

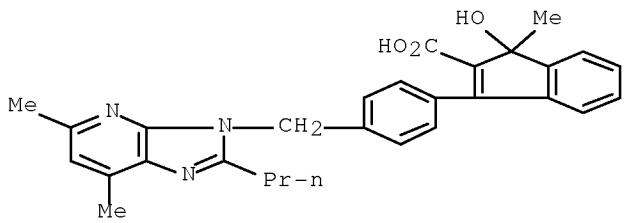
IT Angiotensin AT1 receptor antagonists
Antihypertensives
Pharmacokinetics
Structure-activity relationship
(Further Studies on Imidazo[4,5-b]pyridine AT1 Angiotensin II Receptor Antagonists. Effects of the Transformation of the 4-Phenylquinoline Backbone into 4-Phenylisoquinolinone or 1-Phenylindene Scaffolds)

IT 133240-46-7P 133240-47-8P 155097-12-4P 157553-49-6P 663219-74-7P
700376-02-9P 700376-04-1P 700376-12-1P 700376-13-2P 700376-15-4P
700376-16-5P 700376-17-6P 700376-18-7P 700376-20-1P 700376-22-3P
700376-23-4P 912564-30-8P 912564-31-9P 912564-32-0P 912564-33-1P
912564-34-2P 912564-35-3P 912564-36-4P 912564-37-5P 912564-40-0P
912564-41-1P 912564-42-2P 912564-43-3P 912564-44-4P
912564-57-9P 912564-59-1P 912564-60-4P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(Further Studies on Imidazo[4,5-b]pyridine AT1 Angiotensin II Receptor Antagonists. Effects of the Transformation of the 4-Phenylquinoline Backbone into 4-Phenylisoquinolinone or 1-Phenylindene Scaffolds)

IT 53904-41-9P 94224-68-7P 696661-28-6P 912564-21-7P 912564-23-9P
912564-45-5P 912564-46-6P 912564-47-7P 912564-48-8P 912564-49-9P
912564-50-2P 912564-51-3P 912564-52-4P 912564-53-5P 912564-54-6P
912564-55-7P 912564-56-8P 912564-58-0P 912564-62-6P
912564-63-7P 912564-64-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(Further Studies on Imidazo[4,5-b]pyridine AT1 Angiotensin II Receptor Antagonists. Effects of the Transformation of the 4-Phenylquinoline Backbone into 4-Phenylisoquinolinone or 1-Phenylindene Scaffolds)

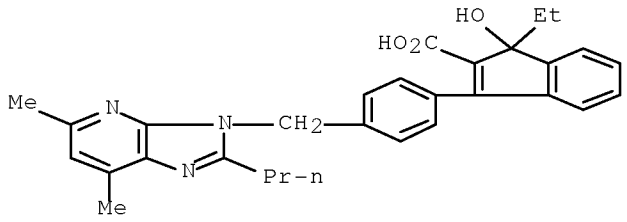
IT 912564-41-1P 912564-42-2P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(Further Studies on Imidazo[4,5-b]pyridine AT1 Angiotensin II Receptor Antagonists. Effects of the Transformation of the 4-Phenylquinoline Backbone into 4-Phenylisoquinolinone or 1-Phenylindene Scaffolds)

RN 912564-41-1 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 3-[4-[(5,7-dimethyl-2-propyl-3H-imidazo[4,5-b]pyridin-3-yl)methyl]phenyl]-1-hydroxy-1-methyl- (CA INDEX NAME)



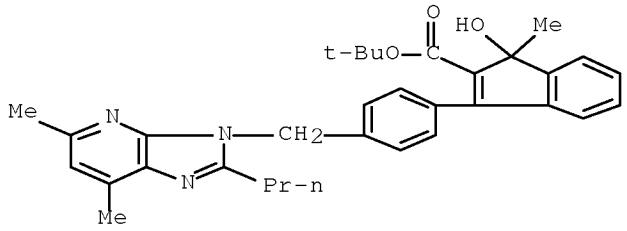
RN 912564-42-2 ZCAPLUS

CN 1H-Indene-2-carboxylic acid, 3-[4-[(5,7-dimethyl-2-propyl-3H-imidazo[4,5-b]pyridin-3-yl)methyl]phenyl]-1-ethyl-1-hydroxy- (CA INDEX NAME)

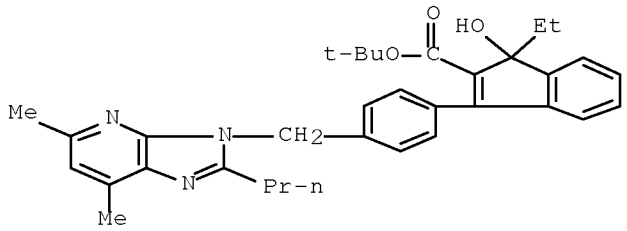


IT 912564-55-7P 912564-56-8P 912564-63-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(Further Studies on Imidazo[4,5-b]pyridine AT1 Angiotensin II Receptor Antagonists. Effects of the Transformation of the 4-Phenylquinoline Backbone into 4-Phenylisoquinolinone or 1-Phenylindene Scaffolds)

RN 912564-55-7 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 3-[4-[(5,7-dimethyl-2-propyl-3H-imidazo[4,5-b]pyridin-3-yl)methyl]phenyl]-1-hydroxy-1-methyl-, 1,1-dimethylethyl ester (CA INDEX NAME)

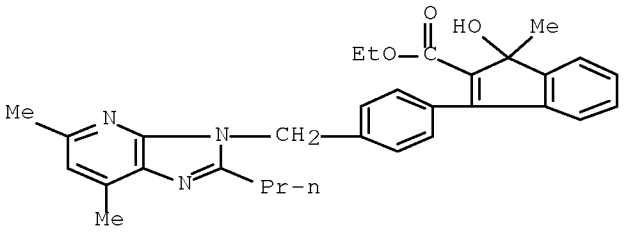


RN 912564-56-8 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 3-[4-[(5,7-dimethyl-2-propyl-3H-imidazo[4,5-b]pyridin-3-yl)methyl]phenyl]-1-ethyl-1-hydroxy-, 1,1-dimethylethyl ester (CA INDEX NAME)



RN 912564-63-7 ZCAPLUS

CN 1H-Indene-2-carboxylic acid, 3-[4-[(5,7-dimethyl-2-propyl-3H-imidazo[4,5-b]pyridin-3-yl)methyl]phenyl]-1-hydroxy-1-methyl-, ethyl ester (CA INDEX NAME)



REFERENCE COUNT: 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L106 ANSWER 8 OF 40 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2006:904051 ZCAPLUS Full-text
DOCUMENT NUMBER: 145:471184
TITLE: 1,4-Addition of arylboronic acids to β-aryl-α,β-unsaturated ketones and esters catalyzed by a rhodium(I)-chiraphos complex for catalytic and enantioselective synthesis of selective endothelin A receptor antagonists
AUTHOR(S): Itoh, Takahiro; Mase, Toshiaki; Nishikata, Takashi; Iyama, Tetsuji; Tachikawa, Hiroto; Kobayashi, Yuri; Yamamoto, Yasunori; Miyaura, Norio
CORPORATE SOURCE: Process R&D, Banyu Pharmaceutical Co. Ltd, Okazaki, Aichi, 4440858, Japan
SOURCE: Tetrahedron (2006), 62(41), 9610-9621
CODEN: TETRAB; ISSN: 0040-4020
PUBLISHER: Elsevier Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 145:471184

AB An enantioselective synthesis of acyclic β-diaryl ketones and esters via 1,4-addition of arylboronic acids to β-aryl-α,β-unsatd. ketones or esters is described. The complex in situ prepared from [Rh(nbd)2]BF4 and chiraphos was found to be an excellent catalyst to achieve high enantioselectivities in a range of 83-89% ee for the ketone derivs. and 78-94% ee for tert-Bu β-arylacrylate derivs. The protocol provided a catalytic method for the enantioselective synthesis of selective endothelin A receptor antagonists (e.g., SB217242) reported by SmithKline Beecham and Merck-Banyu. The enantioselection mechanism and efficiency of the chiraphos ligand for β-aryl-α,β-unsatd. ketones and esters are discussed on the basis of results of DFT computational studies on the modes of coordination of the enone substrates to the phenylrhodium(I)-(S,S)-chiraphos complex.

CC 25-1 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
Section cross-reference(s): 27, 29

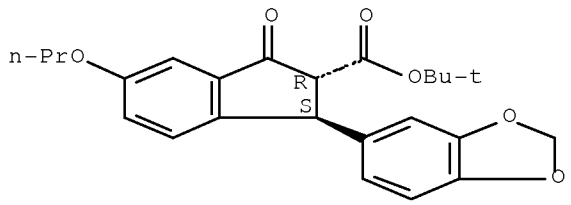
IT 464170-03-4P 464170-07-8P 913648-31-4P 913648-33-6P 913648-35-8P
913648-38-1P 913648-40-5P 913648-42-7P 913648-44-9P
913648-46-1P 913648-48-3P 913648-50-7P 913648-53-0P
913648-54-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)
(1,4-addition of arylboronic acids to β-aryl-α,β-unsatd. ketones and esters catalyzed by a rhodium(I)-chiraphos complex for catalytic and enantioselective synthesis of selective endothelin A receptor antagonists)

IT 913648-44-9P 913648-46-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(1,4-addition of arylboronic acids to β-aryl-α,β-unsatd. ketones and esters catalyzed by a rhodium(I)-chiraphos complex for catalytic and enantioselective synthesis of selective endothelin A receptor antagonists)

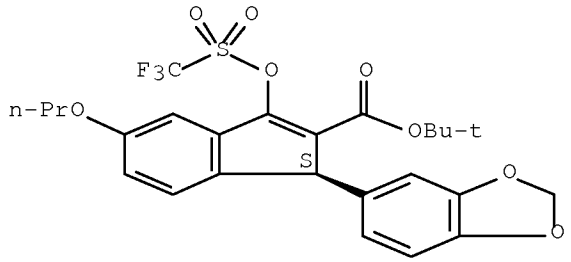
RN 913648-44-9 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-(1,3-benzodioxol-5-yl)-2,3-dihydro-3-oxo-5-propoxy-, 1,1-dimethylethyl ester, (1S,2R)- (CA INDEX NAME)

Absolute stereochemistry.



RN 913648-46-1 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-(1,3-benzodioxol-5-yl)-5-propoxy-3-[[(trifluoromethyl)sulfonyl]oxy]-, 1,1-dimethylethyl ester, (1S)- (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 99 THERE ARE 99 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L106 ANSWER 9 OF 40 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2006:872715 ZCAPLUS Full-text
DOCUMENT NUMBER: 145:454791
TITLE: Synthesis of indenyl ethers by gold(I)-catalyzed intramolecular carboalkoxylation of alkynes
AUTHOR(S): Dube, Pascal; Toste, F. Dean
CORPORATE SOURCE: Department of Chemistry, University of California,

Berkeley, CA, 94720, USA
SOURCE: Journal of the American Chemical Society (2006), 128(37), 12062-12063
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 145:454791

AB The gold(I)-catalyzed carboalkoxylation of alkynes to form indanone derivs. from readily available ortho-acetylenic benzylic ethers is described. Importantly, the gold(I)-catalyzed rearrangement of enantioenriched benzylic ethers proceeds with chirality transfer, thus providing a practical method for the enantioselective synthesis of indenyl ethers.

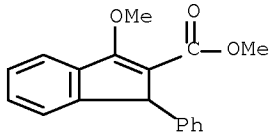
CC 25-9 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)

IT 65684-96-0P 85221-55-2P 913192-73-1P 913192-75-3P
913192-76-4P 913192-77-5P 913192-78-6P
913192-79-7P 913192-80-0P 913192-81-1P 913192-82-2P
913192-91-3P 913192-93-5P 913192-96-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of indenyl ethers via gold-catalyzed intramol. carboalkoxylation of alkynylbenzylic ethers)

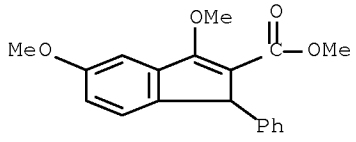
IT 913193-05-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(stereoselective preparation of [(methoxyphenyl)allyl]indenonecarboxylate via gold-catalyzed carboalkoxylation of [allyloxy(methoxyphenyl)methylphenyl]propiolate followed by stereoselective Claisen rearrangement)

IT 913192-75-3P 913192-77-5P 913192-78-6P
913192-79-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of indenyl ethers via gold-catalyzed intramol. carboalkoxylation of alkynylbenzylic ethers)

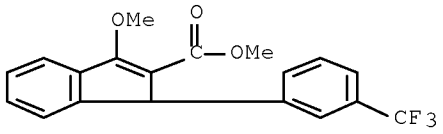
RN 913192-75-3 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 3-methoxy-1-phenyl-, methyl ester (CA INDEX NAME)



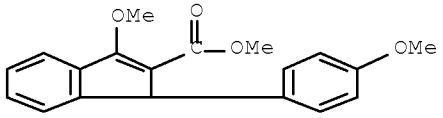
RN 913192-77-5 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 3,5-dimethoxy-1-phenyl-, methyl ester (CA INDEX NAME)



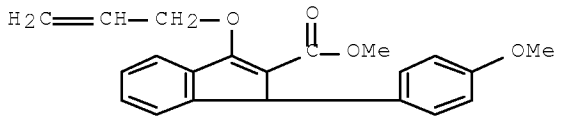
RN 913192-78-6 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 3-methoxy-1-[3-(trifluoromethyl)phenyl]-, methyl ester (CA INDEX NAME)



RN 913192-79-7 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 3-methoxy-1-(4-methoxyphenyl)-, methyl ester (CA INDEX NAME)



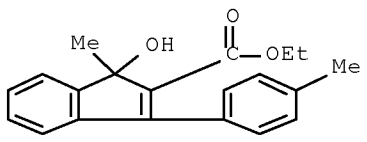
IT 913193-05-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(stereoselective preparation of [(methoxyphenyl)allyl]indenonecarboxylate via gold-catalyzed carboalkoxylation of [allyloxy(methoxyphenyl)methylphenyl]propiolate followed by stereoselective Claisen rearrangement)
RN 913193-05-2 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-(4-methoxyphenyl)-3-(2-propen-1-yloxy)-, methyl ester (CA INDEX NAME)



REFERENCE COUNT: 58 THERE ARE 58 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L106 ANSWER 10 OF 40 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2005:653151 ZCAPLUS Full-text
DOCUMENT NUMBER: 143:306638
TITLE: New π-stacked benzofulvene polymer showing thermoreversible polymerization: Studies in macromolecular and aggregate structures and polymerization mechanism
AUTHOR(S): Cappelli, Andrea; Anzini, Maurizio; Vomero, Salvatore; Donati, Alessandro; Zetta, Lucia; Mendichi, Raniero;

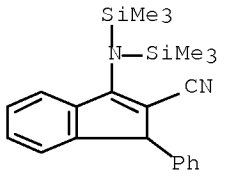
Casolaro, Mario; Lupetti, Pietro; Salvatici, Paolo; Giorgi, Gianluca
CORPORATE SOURCE: Dipartimento Farmaco Chimico Tecnologica and European Research Centre for Drug Discovery and Development, Universita degli Studi di Siena, Siena, 53100, Italy
SOURCE: Journal of Polymer Science, Part A: Polymer Chemistry (2005), 43(15), 3289-3304
CODEN: JPACEC; ISSN: 0887-624X
PUBLISHER: John Wiley & Sons, Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The macromol. and aggregate structures of poly[ethyl 1-methylene-3-(4-methylphenyl)-1H-indene-2-carboxylate] (poly-BF1; a polymer based on a functionalized benzofulvene moiety showing interesting properties, i.e., thermoreversible polymerization/depolymn. behavior, high solubility in the most common organic solvents, and susceptibility to mol. manipulation) have been investigated with NMR spectroscopy, absorption and emission spectrophotometry, and transmission electron microscopy (TEM). Moreover, the polymerization mechanism has been studied to obtain further information on the polymer structure. The collected evidence is consistent in indicating for poly-BF1 a vinyl (1,2) polymer structure stabilized by means of aromatic stacking interactions. Furthermore, TEM studies performed on metal replicas have shown that the polymer is liable to give nanostructured aggregates.
CC 35-4 (Chemistry of Synthetic High Polymers)
IT 637760-42-0, Ethyl 1-hydroxy-1-methyl-3-(4-methylphenyl)-1H-indene-2-carboxylate
RL: RCT (Reactant); RACT (Reactant or reagent)
(monomer precursor; macromol. and aggregate structures and polymerization mechanism in prepn π-stacked benzofulvene polymer showing thermoreversible polymerization)
IT 637760-42-0, Ethyl 1-hydroxy-1-methyl-3-(4-methylphenyl)-1H-indene-2-carboxylate
RL: RCT (Reactant); RACT (Reactant or reagent)
(monomer precursor; macromol. and aggregate structures and polymerization mechanism in prepn π-stacked benzofulvene polymer showing thermoreversible polymerization)
RN 637760-42-0 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-hydroxy-1-methyl-3-(4-methylphenyl)-, ethyl ester (CA INDEX NAME)



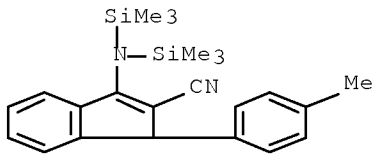
REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L106 ANSWER 11 OF 40 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2004:880443 ZCAPLUS Full-text
DOCUMENT NUMBER: 142:463430
TITLE: Intramolecular cyclization and disilylation of 1,1-dicyano-2,2-diarylethenes promoted by samarium/TMSCl in DMF: a new approach to the syntheses

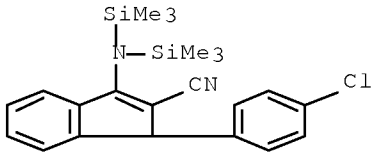
of polysubstituted indenes. [Erratum to document cited in CA141:156911]
AUTHOR(S): Liu, Yongjun; Zhao, Qinliang; Zhang, Yongmin
CORPORATE SOURCE: Department of Chemistry, Zhejiang University, Hangzhouz, 310028, Peop. Rep. China
SOURCE: Tetrahedron Letters (2004), 45(47), 8763
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB In Table 1, several structures of substrate 1 (entries 2-5, 8) were drawn incorrectly. The structures originally published with meta-substitution of the Ph rings should be corrected as their para-isomers. The corrected structures of substrate 1 are given.
CC 25-23 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
IT 731851-22-2P 731851-23-3P 731851-24-4P 731851-25-5P
731851-26-6P 731851-27-7P 731851-28-8P 731851-29-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of polysubstituted indenes via regioselective intramol. cyclization and disilylation of dicyanodiarylethenes promoted by samarium/TMSCl in DMF (Erratum))
IT 731851-22-2P 731851-25-5P 731851-27-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of polysubstituted indenes via regioselective intramol. cyclization and disilylation of dicyanodiarylethenes promoted by samarium/TMSCl in DMF (Erratum))
RN 731851-22-2 ZCAPLUS
CN 1H-Indene-2-carbonitrile, 3-[bis(trimethylsilyl)amino]-1-phenyl- (CA INDEX NAME)



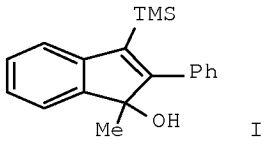
RN 731851-25-5 ZCAPLUS
CN 1H-Indene-2-carbonitrile, 3-[bis(trimethylsilyl)amino]-1-(4-methylphenyl)- (CA INDEX NAME)



RN 731851-27-7 ZCAPLUS
CN 1H-Indene-2-carbonitrile, 3-[bis(trimethylsilyl)amino]-1-(4-chlorophenyl)- (CA INDEX NAME)



L106 ANSWER 12 OF 40 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2004:481984 ZCAPLUS Full-text
DOCUMENT NUMBER: 141:123454
TITLE: Cobalt-catalyzed regioselective carbocyclization reaction of o-iodophenyl ketones and aldehydes with alkynes, acrylates, and acrylonitrile: A facile route to indenols and indenes
AUTHOR(S): Chang, Kuo-Jui; Rayabarapu, Dinesh Kumar; Cheng, Chien-Hong
CORPORATE SOURCE: Department of Chemistry, Tsing Hua University, Hsinchu, Taiwan, 300, Peop. Rep. China
SOURCE: Journal of Organic Chemistry (2004), 69(14), 4781-4787
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 141:123454
GI



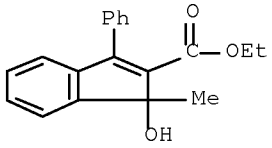
I

AB An efficient cobalt-catalyzed carbocyclization for the synthesis of indenols, e.g., I, and indenes and a method for reductive decyanation are described. 2-Iodophenyl ketones and aldehydes underwent carbocyclization with various disubstituted alkynes, in the presence of Co(dppe)I2 and zinc powder, to afford the corresponding indenol derivs. in good yields. For some unsym. alkynes, the carbocyclization was remarkably regioselective, affording a single regioisomer. The cobalt-catalyzed carbocyclization reaction was successfully extended to the synthesis of indene derivs. Thus, the reaction of 2-iodophenyl ketones and aldehydes with acrylates and acrylonitrile proceeded smoothly, in the presence of Co(dppe)Cl2/dppe and zinc powder, the corresponding indenes in moderate to good yields. Interestingly, when acrylonitrile was employed for the carbocyclization, reductive decyanation also occurred to give an indene derivative without the cyano functionality. A possible mechanism for this cobalt-catalyzed carbocyclization reaction is also proposed.
CC 25-23 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
Section cross-reference(s): 75
IT 222041-16-9P 396688-43-0P 447439-46-5P 447439-55-6P 600735-23-7P

600735-27-1P 617692-10-1P 617692-12-3P 617692-13-4P 617692-14-5P
617692-15-6P 617692-16-7P 724776-29-8P 724776-31-2P
724776-32-3P 724776-33-4P 724776-34-5P 724776-35-6P 724776-36-7P
724776-37-8P 724776-38-9P 724776-39-0P 724776-41-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(regioselective preparation of indenols via cobalt-catalyzed carbocyclization of iodoaryl ketones or iodobenzaldehydes with alkynes)

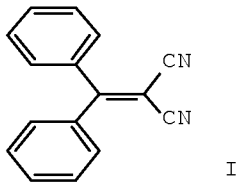
IT 724776-29-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(regioselective preparation of indenols via cobalt-catalyzed carbocyclization of iodoaryl ketones or iodobenzaldehydes with alkynes)

RN 724776-29-8 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-hydroxy-1-methyl-3-phenyl-, ethyl ester (CA INDEX NAME)

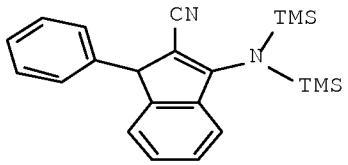


REFERENCE COUNT: 54 THERE ARE 54 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L106 ANSWER 13 OF 40 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2004:403493 ZCAPLUS Full-text
DOCUMENT NUMBER: 141:156911
TITLE: Intramolecular cyclization and disilylation of 1,1-dicyano-2,2-diarylethenes promoted by samarium/TMSCl in DMF: a new approach to the syntheses of polysubstituted indenes
AUTHOR(S): Liu, Yongjun; Zhao, Qinliang; Zhang, Yongmin
CORPORATE SOURCE: Department of Chemistry, Zhejiang University (Campus Xixi), Hangzhou, 310028, Peop. Rep. China
SOURCE: Tetrahedron Letters (2004), 45(23), 4571-4575
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 141:156911
GI



I



II

AB Promoted by samarium metal in DMF and in the presence of TMSCl, 1,1-diaryl-2,2-dicyanoethylenes, e.g. I, undergo an unexpected reductive cyclization simultaneously accompanying with disilylation occurring at the amino moiety resulting from the reduction of the cyano group, which represent a new approach to the construction of indene derivs., e.g. II.

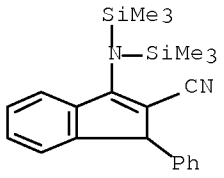
CC 25-23 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)

IT 731851-22-2P 731851-23-3P 731851-24-4P 731851-25-5P
731851-26-6P 731851-27-7P 731851-28-8P 731851-29-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of polysubstituted indenes via regioselective intramol. cyclization and disilylation of dicyanodiarylethenes promoted by samarium/TMSCl in DMF)

IT 731851-22-2P 731851-25-5P 731851-27-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of polysubstituted indenes via regioselective intramol. cyclization and disilylation of dicyanodiarylethenes promoted by samarium/TMSCl in DMF)

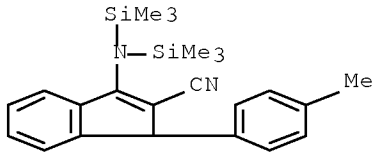
RN 731851-22-2 ZCAPLUS

CN 1H-Indene-2-carbonitrile, 3-[bis(trimethylsilyl)amino]-1-phenyl- (CA INDEX NAME)



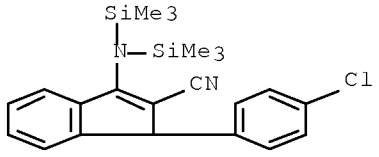
RN 731851-25-5 ZCAPLUS

CN 1H-Indene-2-carbonitrile, 3-[bis(trimethylsilyl)amino]-1-(4-methylphenyl)- (CA INDEX NAME)



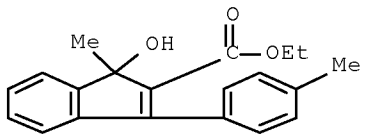
RN 731851-27-7 ZCAPLUS

CN 1H-Indene-2-carbonitrile, 3-[bis(trimethylsilyl)amino]-1-(4-chlorophenyl)- (CA INDEX NAME)



REFERENCE COUNT: 45 THERE ARE 45 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

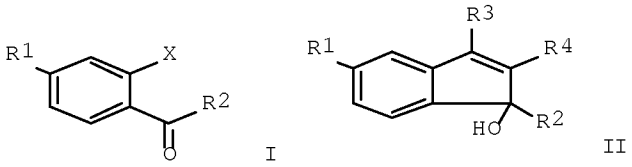
L106 ANSWER 14 OF 40 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2003:851610 ZCAPLUS Full-text
DOCUMENT NUMBER: 140:59976
TITLE: Synthesis and Characterization of a New Benzofulvene Polymer Showing a Thermoreversible Polymerization Behavior
AUTHOR(S): Cappelli, Andrea; Mohr, Galla Pericot; Anzini, Maurizio; Vomero, Salvatore; Donati, Alessandro; Casolaro, Mario; Mendichi, Raniero; Giorgi, Gianluca; Makovec, Francesco
CORPORATE SOURCE: Dipartimento Farmaco Chimico Tecnologico, Universita degli Studi di Siena, Siena, 53100, Italy
SOURCE: Journal of Organic Chemistry (2003), 68(24), 9473-9476
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A new polymer based on a functionalized benzofulvene moiety has been synthesized by spontaneous polymerization of the monomer in the solid state. This polymer shows a very high molar mass, high solubility in the most common organic solvents, and thermoreversible polymerization properties. An interesting application in synthesis is reported.
CC 35-2 (Chemistry of Synthetic High Polymers)
IT 637760-42-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of, and in dehydration synthesis of monomer)
IT 637760-42-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of, and in dehydration synthesis of monomer)
RN 637760-42-0 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-hydroxy-1-methyl-3-(4-methylphenyl)-, ethyl ester (CA INDEX NAME)



REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L106 ANSWER 15 OF 40 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2003:585722 ZCAPLUS Full-text
DOCUMENT NUMBER: 139:261025
TITLE: Regioselective Synthesis of Indenols via Nickel-Catalyzed Carbocyclization Reaction
AUTHOR(S): Rayabarapu, Dinesh Kumar; Yang, Chun-Hui; Cheng, Chien-Hong
CORPORATE SOURCE: Department of Chemistry, Tsing Hua University,

Hsinchu, 300, Taiwan
SOURCE: Journal of Organic Chemistry (2003), 68(17), 6726-6731
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 139:261025
GI



AB 2-Halophenyl ketones I (1a-1e: 1a, o-IC6H4COCH3; 1b, o-BrC6H4COCH3, etc.) undergo carbocyclization with alkyl propiolates R3C.tplbond.R4 (2a, CH3(CH2)4C.tplbond.CCO2CH3; 2b, TMSC.tplbond.CCO2Et; 2c, CH3C.tplbond.CCO2CH3; 2d, CH3OCH2C.tplbond.CCO2CH3; 2e, CH3(CH2)3C.tplbond.CCO2CH3; 2f, PhC.tplbond.CCO2CH3; and 2g, Me3C.tplbond.CCO2CH3) in the presence of Ni(dppe)Br2 and Zn powder in MeCN at 80° to afford the corresponding indenol derivs. II with remarkable regioselectivity in good to excellent yields. The Ni-catalyzed carbocyclization reaction was successfully extended to other simple disubstituted alkynes. Thus, the reaction of 2-halophenyl ketones I with disubstituted alkynes (2h, PhC.tplbond.CPh; 2i, CH3C6H4C.tplbond.CC6H4CH3; 2j, CH3CH2C.tplbond.CCH2CH3; 2k, PhC.tplbond.CCH3; 2l, TMSC.tplbond.CCH3; and 2m, PhC.tplbond.C(CH2)3CH3) proceeded smoothly to afford the corresponding indenols in good to excellent yields. For unsym. alkynes 2k-m, the carbocyclization gave two regioisomers with regioselectivities ranging from 1:2 to 1:12 depending on the substituents on the alkyne and on the aromatic ring of halophenyl ketone. A possible mechanism for this Ni-catalyzed carbocyclization reaction is also proposed.

CC 25-23 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)

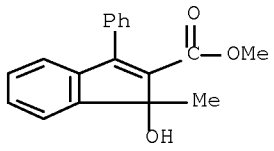
IT 5418-21-3P 117583-04-7P 222041-16-9P 222041-22-7P 447439-45-4P
447439-46-5P 447439-47-6P 447439-48-7P 447439-49-8P
447439-50-1P 447439-51-2P 447439-52-3P 447439-53-4P
447439-54-5P 447439-55-6P 447439-56-7P 447439-57-8P
447439-59-0P 600735-10-2P 600735-11-3P 600735-12-4P 600735-13-5P
600735-14-6P 600735-15-7P 600735-16-8P 600735-17-9P 600735-18-0P
600735-19-1P 600735-20-4P 600735-21-5P 600735-22-6P 600735-23-7P
600735-24-8P 600735-25-9P 600735-26-0P 600735-27-1P 600735-28-2P
600735-29-3P 600735-30-6P 600735-31-7P 600735-32-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(regioselective nickel-catalyzed carbocyclization of o-halophenyl ketones with alkyl propiolates or disubstituted alkynes to give indenols)

IT 447439-50-1P 447439-57-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(regioselective nickel-catalyzed carbocyclization of o-halophenyl ketones with alkyl propiolates or disubstituted alkynes to give indenols)

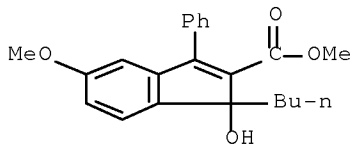
RN 447439-50-1 ZCAPLUS

CN 1H-Indene-2-carboxylic acid, 1-hydroxy-1-methyl-3-phenyl-, methyl ester

(CA INDEX NAME)



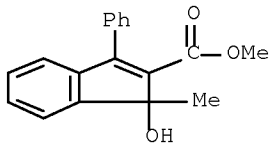
RN 447439-57-8 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-butyl-1-hydroxy-5-methoxy-3-phenyl-, methyl ester (CA INDEX NAME)



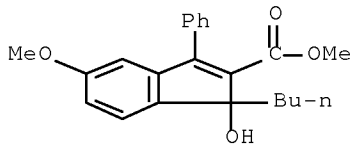
REFERENCE COUNT: 48 THERE ARE 48 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L106 ANSWER 16 OF 40 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2002:314156 ZCAPLUS Full-text
DOCUMENT NUMBER: 137:169301
TITLE: Nickel-catalyzed regioselective carbocyclization of ortho-halophenyl ketones with propiolates: an efficient route to disubstituted indenols
AUTHOR(S): Rayabarapu, Dinesh Kumar; Cheng, Chien-Hong
CORPORATE SOURCE: Department of Chemistry, Tsing Hua University, Hsinchu, 300, Taiwan
SOURCE: Chemical Communications (Cambridge, United Kingdom) (2002), (9), 942-943
CODEN: CHCOFS; ISSN: 1359-7345
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 137:169301
AB Carbocylization of o-halophenyl ketones with propiolates in the presence of Ni(dppe)Br2 and Zn powder in MeCN at 80° afforded the corresponding 2,3-disubstituted indenols.
CC 25-23 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
IT 447439-45-4P 447439-46-5P 447439-48-7P 447439-49-8P
447439-50-1P 447439-51-2P 447439-52-3P 447439-53-4P
447439-54-5P 447439-55-6P 447439-56-7P 447439-57-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of indenols by nickel-catalyzed regioselective cyclization of o-halophenyl ketones with propiolates)
IT 447439-50-1P 447439-57-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of indenols by nickel-catalyzed regioselective cyclization of o-halophenyl ketones with propiolates)

RN 447439-50-1 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-hydroxy-1-methyl-3-phenyl-, methyl ester (CA INDEX NAME)

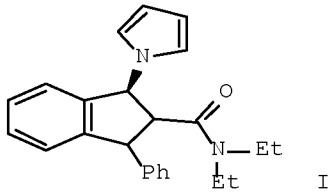


RN 447439-57-8 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-butyl-1-hydroxy-5-methoxy-3-phenyl-, methyl ester (CA INDEX NAME)



REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L106 ANSWER 17 OF 40 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2002:106231 ZCAPLUS Full-text
DOCUMENT NUMBER: 137:78743
TITLE: Synthesis of a Novel Class of Non-Peptide NK-2 Receptor Ligand, Derived from 1-Phenyl-3-pyrrol-1-ylindan-2-carboxamides
AUTHOR(S): Guillon, Jean; Dallemagne, Patrick; Leger, Jean-Michel; Sopkova, Jana; Bovy, Philippe R.; Jarry, Christian; Rault, Sylvain
CORPORATE SOURCE: EA 2962-Pharmacochimie, UFR des Sciences Pharmaceutiques, Universite Victor Segalen Bordeaux 2, Bordeaux, 33076, Fr.
SOURCE: Bioorganic & Medicinal Chemistry (2002), 10(4), 1043-1050
CODEN: BMECEP; ISSN: 0968-0896
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 137:78743
GI



I

AB A series of trans,trans-1-phenyl-3-pyrrol-1-ylindan-2-carboxamide derivs., e.g., I, has been synthesized in eight steps starting from cinnamic acid or 3,3-diphenylpropionic acid. The trans,trans configuration of these carboxamides has been established by X-ray anal. and by NOE expts. in NMR. These new compds. were evaluated for their potential NK-1, NK-2 and NK-3 receptors binding affinity. The N,N-disubstituted carboxamides bound selectively on NK-2 receptors.

CC 25-23 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
Section cross-reference(s): 1, 27

IT 440115-19-5P
RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(stereoselective preparation, crystal structure, tachykinin receptor binding affinity and structure-activity relationship of pyrrolylindancarboxamides as selective NK-2 receptor ligands)

IT 245124-51-0P
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(stereoselective preparation, crystal structure, tachykinin receptor binding affinity and structure-activity relationship of pyrrolylindancarboxamides as selective NK-2 receptor ligands)

IT 440115-07-1P 440115-11-7P 440115-15-1P
440115-22-0P 440115-27-5P 440115-32-2P
440115-36-6P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(stereoselective preparation, tachykinin receptor binding affinity and structure-activity relationship of pyrrolylindancarboxamides as selective NK-2 receptor ligands)

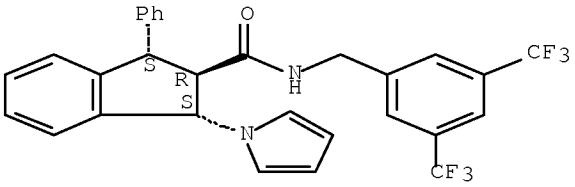
IT 16618-72-7P 245124-53-2P 245124-54-3P
245124-55-4P 245124-56-5P 245124-57-6P
440114-83-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(stereoselective preparation, tachykinin receptor binding affinity and structure-activity relationship of pyrrolylindancarboxamides as selective NK-2 receptor ligands)

IT 440115-19-5P
RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(stereoselective preparation, crystal structure, tachykinin receptor binding affinity and structure-activity relationship of pyrrolylindancarboxamides as selective NK-2 receptor ligands)

RN 440115-19-5 ZCAPLUS

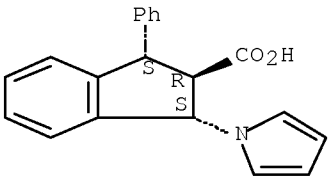
CN 1H-Indene-2-carboxamide, N-[[3,5-bis(trifluoromethyl)phenyl]methyl]-2,3-dihydro-1-phenyl-3-(1H-pyrrol-1-yl)-, (1R,2S,3R)-rel- (CA INDEX NAME)

Relative stereochemistry.



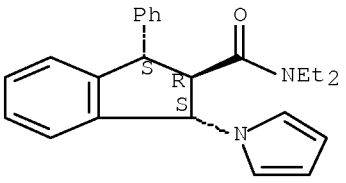
IT 245124-51-0P
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(stereoselective preparation, crystal structure, tachykinin receptor binding
affinity and structure-activity relationship of pyrrolylindancarboxamides as selective NK-2 receptor ligands)
RN 245124-51-0 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 2,3-dihydro-1-phenyl-3-(1H-pyrrol-1-yl)-, (1R,2S,3R)-rel- (CA INDEX NAME)

Relative stereochemistry.



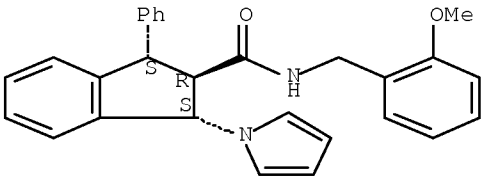
IT 440115-07-1P 440115-15-1P 440115-22-0P
440115-27-5P 440115-32-2P 440115-36-6P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(stereoselective preparation, tachykinin receptor binding affinity and structure-activity relationship of pyrrolylindancarboxamides as selective NK-2 receptor ligands)
RN 440115-07-1 ZCAPLUS
CN 1H-Indene-2-carboxamide, N,N-diethyl-2,3-dihydro-1-phenyl-3-(1H-pyrrol-1-yl)-, (1R,2S,3R)-rel- (CA INDEX NAME)

Relative stereochemistry.



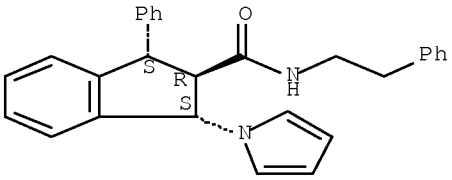
RN 440115-15-1 ZCAPLUS
CN 1H-Indene-2-carboxamide, 2,3-dihydro-N-[(2-methoxyphenyl)methyl]-1-phenyl-3-(1H-pyrrol-1-yl)-, (1R,2S,3R)-rel- (CA INDEX NAME)

Relative stereochemistry.



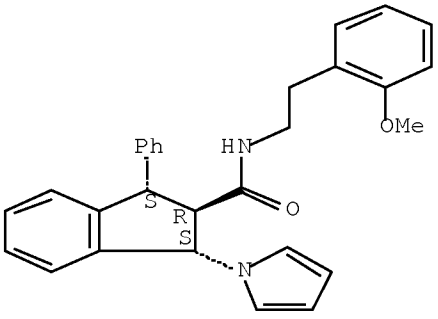
RN 440115-22-0 ZCAPLUS
CN 1H-Indene-2-carboxamide, 2,3-dihydro-1-phenyl-N-(2-phenylethyl)-3-(1H-pyrrol-1-yl)-, (1R,2S,3R)-rel- (CA INDEX NAME)

Relative stereochemistry.



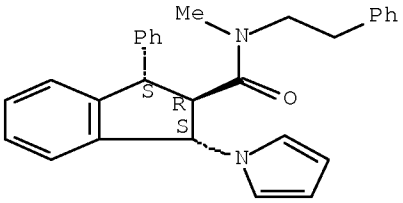
RN 440115-27-5 ZCAPLUS
CN 1H-Indene-2-carboxamide, 2,3-dihydro-N-[2-(2-methoxyphenyl)ethyl]-1-phenyl-3-(1H-pyrrol-1-yl)-, (1R,2S,3R)-rel- (CA INDEX NAME)

Relative stereochemistry.



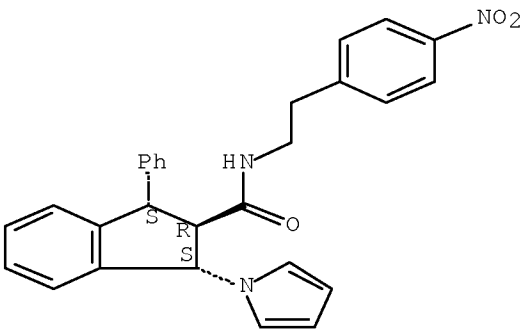
RN 440115-32-2 ZCAPLUS
CN 1H-Indene-2-carboxamide, 2,3-dihydro-N-methyl-1-phenyl-N-(2-phenylethyl)-3-(1H-pyrrol-1-yl)-, (1R,2S,3R)-rel- (CA INDEX NAME)

Relative stereochemistry.

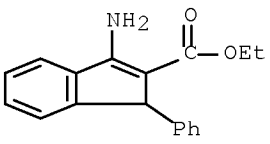


RN 440115-36-6 ZCAPLUS
CN 1H-Indene-2-carboxamide, 2,3-dihydro-N-[2-(4-nitrophenyl)ethyl]-1-phenyl-3-(1H-pyrrol-1-yl)-, (1R,2S,3R)-rel- (CA INDEX NAME)

Relative stereochemistry.

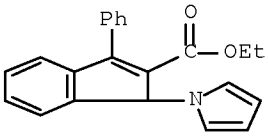


IT 245124-53-2P 245124-54-3P 245124-55-4P
245124-56-5P 245124-57-6P 440114-83-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(stereoselective preparation, tachykinin receptor binding affinity and structure-activity relationship of pyrrolylindancarboxamides as selective NK-2 receptor ligands)
RN 245124-53-2 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 3-amino-1-phenyl-, ethyl ester (CA INDEX NAME)



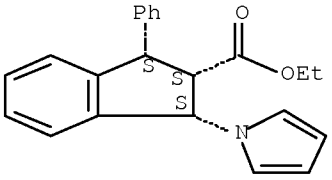
RN 245124-54-3 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 3-phenyl-1-(1H-pyrrol-1-yl)-, ethyl ester

(CA INDEX NAME)

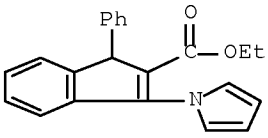


RN 245124-55-4 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 2,3-dihydro-1-phenyl-3-(1H-pyrrol-1-yl)-, ethyl ester, (1R,2R,3R)-rel- (CA INDEX NAME)

Relative stereochemistry.

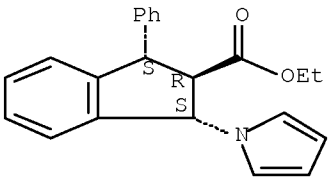


RN 245124-56-5 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-phenyl-3-(1H-pyrrol-1-yl)-, ethyl ester (CA INDEX NAME)



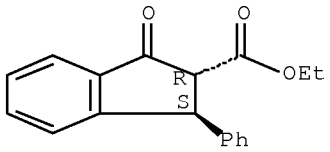
RN 245124-57-6 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 2,3-dihydro-1-phenyl-3-(1H-pyrrol-1-yl)-, ethyl ester, (1R,2S,3R)-rel- (CA INDEX NAME)

Relative stereochemistry.



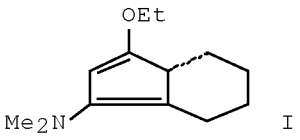
RN 440114-83-0 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 2,3-dihydro-1-oxo-3-phenyl-, ethyl ester, (2R,3S)-rel- (CA INDEX NAME)

Relative stereochemistry.

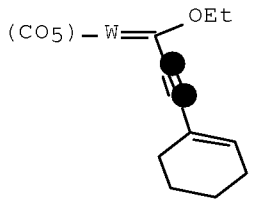


REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L106 ANSWER 18 OF 40 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2001:917587 ZCAPLUS Full-text
DOCUMENT NUMBER: 136:340418
TITLE: Organic synthesis via transition metal complexes, part 113. Highly selective formation of [4+2] and [4+3] cycloadducts of tetrahydroindenes generated in situ from a (1-alkynyl)carbene tungsten complex by the metalla-1,3,5-hexatriene route
AUTHOR(S): Wu, He-Ping; Aumann, Rudolf; Frohlich, Roland; Wibbeling, Birgit; Kataeva, Olga
CORPORATE SOURCE: Organisch-Chemisches Institut der Universitat Munster, Munster, 48149, Germany
SOURCE: Chemistry--A European Journal (2001), 7(23), 5084-5093 CODEN: CEUJED; ISSN: 0947-6539
PUBLISHER: Wiley-VCH Verlag GmbH
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 136:340418
GI



I



II

AB 1-Amino-3-ethoxytetrahydro-3aH-indenes, e.g. I, can be readily generated together with pentacarbonyl(pyridine)tungsten in a template induced three-component reaction of [(1-cyclohexenyl)ethynyl]carbene tungsten complex II with secondary amines and pyridine. Even though the compds. I are thermally quite unstable and undergo a fast rearrangement to tetrahydro-7aH-indenes, they can be trapped by formation of (rather strained) [4+2] cycloadducts with maleimide. If 1-amino-3- ethoxytetrahydro-3aH-indenes I are generated in the presence of electron-poor alkynes, they undergo a 1,5-shift to give

tetrahydro-7aH-indenes, which in turn afford [4+2] cycloadducts. Condensation of 1-tungsta-1,3,5-hexatrienes (3E)-5a-d with 1-metalla-1,3-butadienes (M = Cr, W) give [4+3] cycloadducts of tetrahydro-7aH-indenes in good yields with high regio- and stereoselectivity.

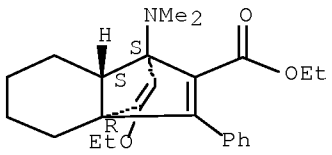
CC 24-8 (Alicyclic Compounds)
Section cross-reference(s): 29

IT 415725-56-3P 415725-58-5P 415725-59-6P
415725-60-9P 415725-61-0P 415725-62-1P 415725-63-2P 415725-70-1P
415725-71-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(selective formation of [4+2] and [4+3] cycloa-adducts of tetrahydroindenes generated in situ from a (1-alkynyl)carbene tungsten complex by the metalla-1,3,5-hexatriene route)

IT 415725-56-3P 415725-58-5P 415725-59-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(selective formation of [4+2] and [4+3] cycloa-adducts of tetrahydroindenes generated in situ from a (1-alkynyl)carbene tungsten complex by the metalla-1,3,5-hexatriene route)

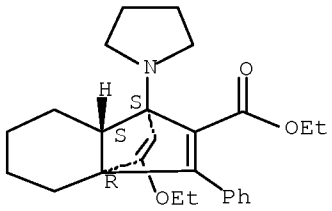
RN 415725-56-3 ZCAPLUS
CN 1,3a-Etheno-3aH-indene-2-carboxylic acid, 1-(dimethylamino)-8-ethoxy-1,4,5,6,7,7a-hexahydro-3-phenyl-, ethyl ester, (1R,3aS,7aR)-rel- (CA INDEX NAME)

Relative stereochemistry.



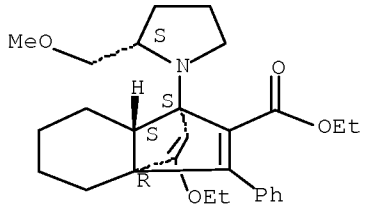
RN 415725-58-5 ZCAPLUS
CN 1,3a-Etheno-3aH-indene-2-carboxylic acid, 8-ethoxy-1,4,5,6,7,7a-hexahydro-3-phenyl-1-(1-pyrrolidinyl)-, ethyl ester, (1R,3aS,7aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 415725-59-6 ZCAPLUS
CN 1,3a-Etheno-3aH-indene-2-carboxylic acid, 8-ethoxy-1,4,5,6,7,7a-hexahydro-1-[(2S)-2-(methoxymethyl)-1-pyrrolidinyl]-3-phenyl-, ethyl ester, (1S,3aR,7aS)- (9CI) (CA INDEX NAME)

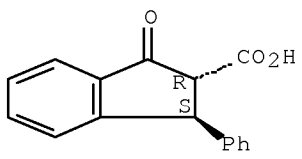
Absolute stereochemistry.



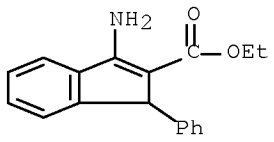
REFERENCE COUNT: 43 THERE ARE 43 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L106 ANSWER 19 OF 40 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1999:516276 ZCAPLUS Full-text
DOCUMENT NUMBER: 131:257401
TITLE: First synthesis of 1-phenyl-3-pyrrol-1-ylindan-2-carboxylic acid, a new scaffold of potential non-peptide endothelin receptor antagonists
AUTHOR(S): Guillon, Jean; Dallemagne, Patrick; Stiebing, Silvia; Bovy, Philippe R.; Rault, Sylvian
CORPORATE SOURCE: Syntheval, Caen, F-14032, Fr.
SOURCE: Synlett (1999), (8), 1263-1264
CODEN: SYNLES; ISSN: 0936-5214
PUBLISHER: Georg Thieme Verlag
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 131:257401
AB The synthesis of trans,trans-1-phenyl-3-pyrrol-1-ylindan-2-carboxylate, a key-intermediate in the access to potential non-peptide endothelin receptor antagonists, is reported.
CC 27-10 (Heterocyclic Compounds (One Hetero Atom))
IT 16618-72-7P 245124-52-1P 245124-53-2P
245124-54-3P 245124-55-4P 245124-56-5P
245124-57-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of phenylpyrrolylindancarboxylate)
IT 245124-51-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of phenylpyrrolylindancarboxylate)
IT 245124-52-1P 245124-53-2P 245124-54-3P
245124-55-4P 245124-56-5P 245124-57-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of phenylpyrrolylindancarboxylate)
RN 245124-52-1 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 2,3-dihydro-1-oxo-3-phenyl-, (2R,3S)-rel- (CA INDEX NAME)

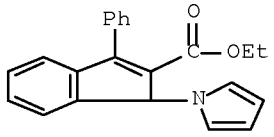
Relative stereochemistry.



RN 245124-53-2 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 3-amino-1-phenyl-, ethyl ester (CA INDEX NAME)

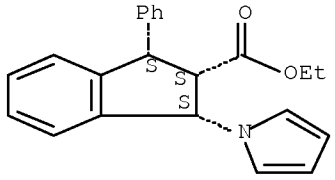


RN 245124-54-3 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 3-phenyl-1-(1H-pyrrol-1-yl)-, ethyl ester (CA INDEX NAME)

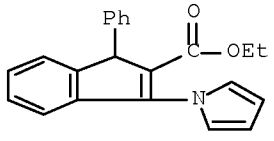


RN 245124-55-4 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 2,3-dihydro-1-phenyl-3-(1H-pyrrol-1-yl)-, ethyl ester, (1R,2R,3R)-rel- (CA INDEX NAME)

Relative stereochemistry.

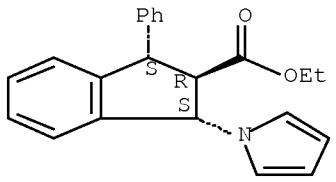


RN 245124-56-5 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-phenyl-3-(1H-pyrrol-1-yl)-, ethyl ester (CA INDEX NAME)



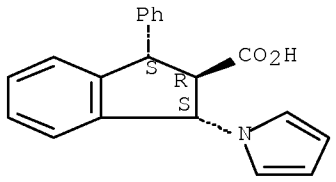
RN 245124-57-6 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 2,3-dihydro-1-phenyl-3-(1H-pyrrol-1-yl)-, ethyl ester, (1R,2S,3R)-rel- (CA INDEX NAME)

Relative stereochemistry.



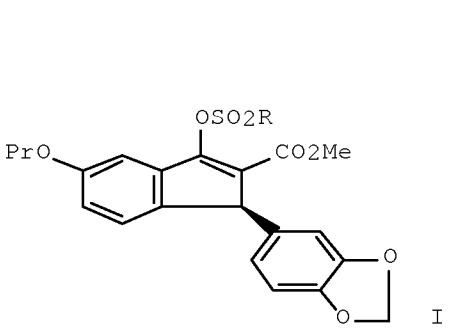
IT 245124-51-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of phenylpyrrolylindancarboxylate)
RN 245124-51-0 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 2,3-dihydro-1-phenyl-3-(1H-pyrrol-1-yl)-, (1R,2S,3R)-rel- (CA INDEX NAME)

Relative stereochemistry.

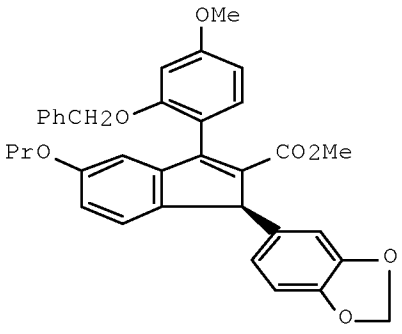


REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L106 ANSWER 20 OF 40 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1998:713120 ZCAPLUS Full-text
DOCUMENT NUMBER: 130:52356
TITLE: An optimized palladium catalyzed cross-coupling of nonracemic trifluoromethylsulfonyl and fluorosulfonyl enol ethers to arylboronic acids
AUTHOR(S): Pridgen, Lendon N.; Huang, G. Kris
CORPORATE SOURCE: Synthetic Chem. Dep., Chemical R & D, SmithKline Beecham Pharmaceuticals, King of Prussia, PA, 19406-0939, USA
SOURCE: Tetrahedron Letters (1998), 39(46), 8421-8424
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I



II

AB Nonracemic enol ethers, e.g., I (R = CF3, F), were cross-coupled to arylboronic acids under palladium [PdCl2(dppf)] catalysis to provide in high yield (>98%) selected 1,3-diarylindenes, e.g., II.

CC 28-5 (Heterocyclic Compounds (More Than One Hetero Atom))

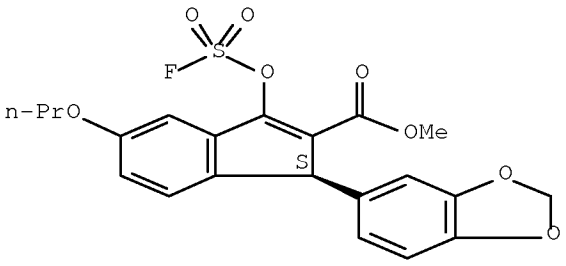
IT 98-80-6, Phenylboronic acid 183474-19-3 183474-23-9
190969-67-6 217307-17-0 217307-18-1 217307-19-2
217307-21-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(palladium catalyzed cross-coupling of nonracemic trifluoromethylsulfonyl and fluorosulfonyl enol ethers to arylboronic acids)

IT 190969-67-6 217307-19-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(palladium catalyzed cross-coupling of nonracemic trifluoromethylsulfonyl and fluorosulfonyl enol ethers to arylboronic acids)

RN 190969-67-6 ZCAPLUS

CN 1H-Indene-2-carboxylic acid, 1-(1,3-benzodioxol-5-yl)-3-[(fluorosulfonyl)oxy]-5-propoxy-, methyl ester, (1S)- (CA INDEX NAME)

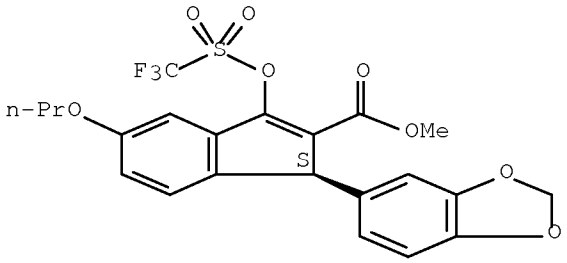
Absolute stereochemistry.



RN 217307-19-2 ZCAPLUS

CN 1H-Indene-2-carboxylic acid, 1-(1,3-benzodioxol-5-yl)-5-propoxy-3-[[(trifluoromethyl)sulfonyl]oxy]-, methyl ester, (1S)- (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 46 THERE ARE 46 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L106 ANSWER 21 OF 40 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1998:650045 ZCAPLUS Full-text
DOCUMENT NUMBER: 129:289939
ORIGINAL REFERENCE NO.: 129:59091a,59094a
TITLE: Indanecarboxylic acid derivatives and their use as endothelin receptor antagonists
INVENTOR(S): Cousins, Russell Donovan; Elliott, John Duncan; Lago, Maria Amparo; Leber, Jack Dale; Peishoff, Catherine Elizabeth
PATENT ASSIGNEE(S): USA
SOURCE: U.S., 30 pp., Cont.-in-part of U.S. Ser. No. 66,818, abandoned.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 4
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5817693	A	19981006	US 1994-336444	19941109
CZ 287406	B6	20001115	CZ 1994-1109	19921029
ZA 9208467	A	19930505	ZA 1992-8467	19921103
ES 2062927	A1	19941216	ES 1992-2548	19921217
ES 2062927	B1	19950701		
US 5716984	A	19980210	US 1995-442038	19950516
US 5719182	A	19980217	US 1995-442443	19950516
US 5716985	A	19980210	US 1995-450938	19950523
US 5719183	A	19980217	US 1995-459686	19950602
US 6271399	B1	20010807	US 1995-459985	19950602
CA 2236924	A1	19970515	CA 1996-2236924	19961108
US 6087389	A	20000711	US 1998-99373	19980618
US 6274737	B1	20010814	US 2000-574413	20000519
US 20020002177	A1	20020103	US 2001-901951	20010710
US 6448260	B2	20020910		

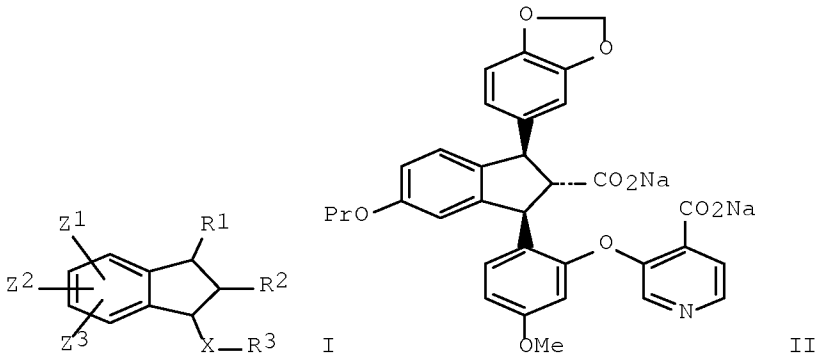
PRIORITY APPLN. INFO.:

US 1991-787870	B2	19911105
US 1992-854195	B2	19920320
US 1993-66818	B2	19930427
CS 1994-1109	A	19921029
WO 1992-US9427	A2	19921029
WO 1994-US4603	A2	19940426
US 1994-336444	A1	19941109
US 1998-99373	A3	19980618

US 2000-574413 A3 20000519

OTHER SOURCE(S): MARPAT 129:289939

GI



AB Novel indane and indene derivs. are described which are endothelin receptor antagonists. In particular, indane derivs. I [R1 = X(CH2)nAr, dihydrobenzofuranyl, benzodioxanyl, cyclohexyl, or aryl; Ar = (un)substituted Ph with certain optional ring fusions, or pyridyl; n = 0-6; R2 = CO2H, CH2CO2H or its α-(di)alkyl derivs., tetrazolyl; R3 = groups given for Ar, NHAc, alkylthio, -sulfinyl, or -sulfonyl; X = (CH2)n or O; Z1-Z3 = H, OH, CH2Ph, alkoxy, amino, alkyl, halo, alkylenedioxy, etc.; with provisos and several specific exclusions] are claimed, as well as their pharmaceutical compns., methods of use, and preparation Claimed uses of I include treatment of hypertension, renal failure, and cerebrovascular disease, including migraine. For instance, a derivative of Me 3-(2-hydroxyphenyl)indane-2-carboxylate underwent a sequence of (1) etherification with 3-fluoro-4-formylpyridine, (2) oxidation of formyl to carboxy, and (3) alkaline saponification of the ester, to give the racemic diastereomeric title salt II. In a [125I]-ET-1 binding protocol using rat cerebellum ETA and ETB receptors in vitro, compds. I gave IC50 values in a range from 0.01 nM to 50 μM.

IC ICM A61K031-36
ICS C07D317-54

INCL 514464000

CC 25-23 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
Section cross-reference(s): 1

ST indanecarboxylate prepn antihypertensive treatment renal failure; cerebrovascular disease treatment indanecarboxylate prepn; endothelin receptor antagonist indanecarboxylate prepn

IT Artery, disease
(coronary, restenosis, treatment or prevention; preparation of indanecarboxylic acid derivs. as endothelin receptor antagonists)

IT Antihypertensives
Antimigraine agents
(preparation of indanecarboxylic acid derivs. as endothelin receptor antagonists)

IT 167084-46-0P 190965-53-8P
RL: PUR (Purification or recovery); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of indanecarboxylic acid derivs. as endothelin receptor antagonists)

IT 167084-47-1P 214271-75-7P

RL: PUR (Purification or recovery); SPN (Synthetic preparation); PREP (Preparation)
(intermediate; preparation of indanecarboxylic acid derivs. as endothelin receptor antagonists)

IT 1462-37-9P 34068-01-4P 63604-94-4P 81729-00-2P 121704-77-6P
133730-24-2P 150356-18-6P 150356-19-7P 150356-20-0P
150356-22-2P 150356-23-3P 150356-24-4P
150356-25-5P 150356-26-6P 150356-27-7P 150356-28-8P
150356-29-9P 150356-30-2P 150356-31-3P 150356-32-4P
150356-33-5P 150356-34-6P 150356-35-7P 150356-36-8P
150356-37-9P 150356-38-0P 150356-39-1P 150356-40-4P
150356-41-5P 150356-42-6P 150356-43-7P 150356-44-8P
150356-45-9P 150356-46-0P 150356-47-1P 150356-48-2P
150356-49-3P 150356-50-6P 150356-51-7P 150356-52-8P
150356-53-9P 150356-54-0P 150356-55-1P 150356-56-2P
150356-57-3P 150356-58-4P 150356-59-5P 150356-60-8P
150356-61-9P 150356-62-0P 150356-68-6P 150356-71-1P
150356-72-2P 150356-73-3P 150356-74-4P 150356-75-5P 150356-76-6P
150356-77-7P 150408-20-1P 156023-58-4P 156129-15-6P 167084-50-6P
167084-51-7P 167084-52-8P 167084-53-9P 167084-54-0P 167084-55-1P
167084-56-2P 167084-57-3P 167256-04-4P 167256-05-5P 190969-68-7P
214271-70-2P 214271-73-5P 214271-80-4P 214271-81-5P
214271-84-8P 214271-85-9P 214271-86-0P 214271-88-2P 214271-89-3P
214271-90-6P 214271-93-9P 214271-96-2P 214271-98-4P 214271-99-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of indanecarboxylic acid derivs. as endothelin receptor antagonists)

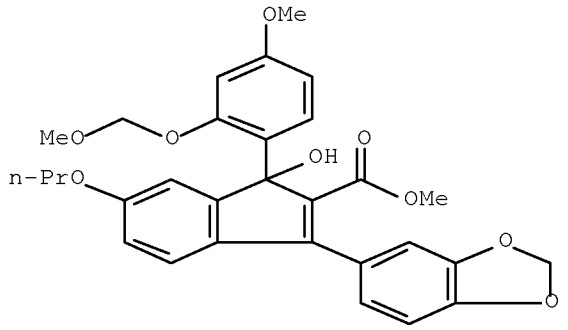
IT 156023-59-5P 214271-74-6P
RL: PEP (Physical, engineering or chemical process); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)
(resolution; preparation of indanecarboxylic acid derivs. as endothelin receptor antagonists)

IT 167084-46-0P
RL: PUR (Purification or recovery); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of indanecarboxylic acid derivs. as endothelin receptor antagonists)

RN 167084-46-0 ZCAPLUS

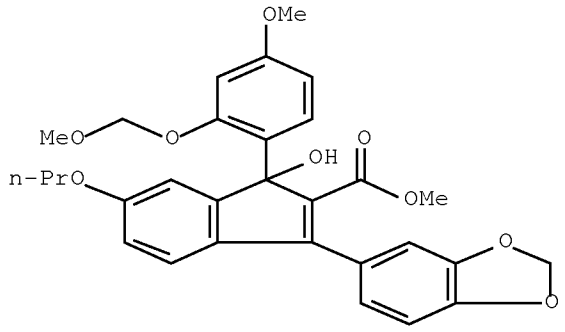
CN 1H-Indene-2-carboxylic acid, 3-(1,3-benzodioxol-5-yl)-1-hydroxy-1-[4-methoxy-2-(methoxymethoxy)phenyl]-6-propoxy-, methyl ester, (+)- (CA INDEX NAME)

Rotation (+).

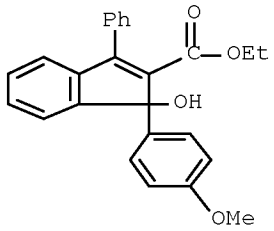


IT 167084-47-1P
RL: PUR (Purification or recovery); SPN (Synthetic preparation); PREP (Preparation)
(intermediate; preparation of indanecarboxylic acid derivs. as endothelin receptor antagonists)
RN 167084-47-1 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 3-(1,3-benzodioxol-5-yl)-1-hydroxy-1-[4-methoxy-2-(methoxymethoxy)phenyl]-6-propoxy-, methyl ester, (-)- (CA INDEX NAME)

Rotation (-).

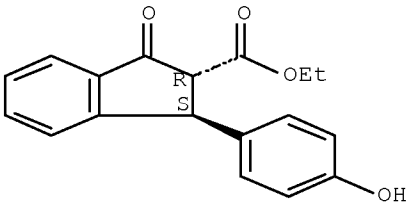


IT 150356-18-6P 150356-22-2P 150356-23-3P
150356-25-5P 150356-33-5P 150356-36-8P
150356-38-0P 150356-41-5P 150356-45-9P
150356-50-6P 150356-55-1P 150356-57-3P
150356-61-9P 214271-73-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of indanecarboxylic acid derivs. as endothelin receptor antagonists)
RN 150356-18-6 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-hydroxy-1-(4-methoxyphenyl)-3-phenyl-, ethyl ester (CA INDEX NAME)



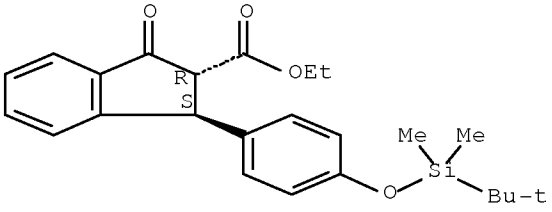
RN 150356-22-2 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 2,3-dihydro-1-(4-hydroxyphenyl)-3-oxo-, ethyl ester, (1R,2S)-rel- (CA INDEX NAME)

Relative stereochemistry.

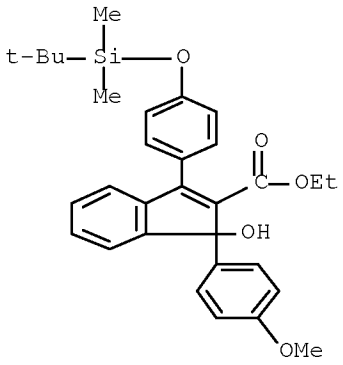


RN 150356-23-3 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-[4-[[(1,1-dimethylethyl)dimethylsilyl]oxy]phenyl]-2,3-dihydro-3-oxo-, ethyl ester, (1R,2S)-rel- (CA INDEX NAME)

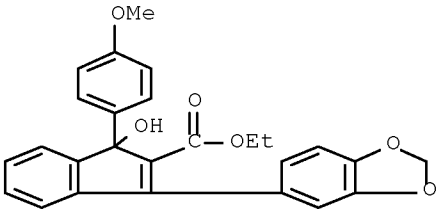
Relative stereochemistry.



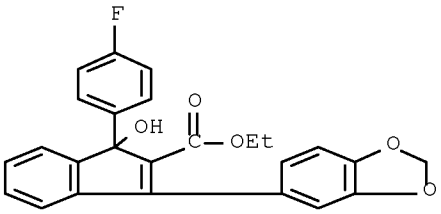
RN 150356-25-5 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 3-[4-[[(1,1-dimethylethyl)dimethylsilyl]oxy]phenyl]-1-hydroxy-1-(4-methoxyphenyl)-, ethyl ester (CA INDEX NAME)



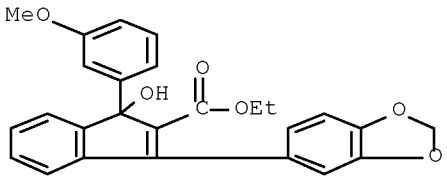
RN 150356-33-5 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 3-(1,3-benzodioxol-5-yl)-1-hydroxy-1-(4-methoxyphenyl)-, ethyl ester (CA INDEX NAME)



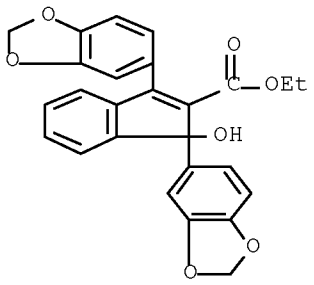
RN 150356-36-8 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 3-(1,3-benzodioxol-5-yl)-1-(4-fluorophenyl)-1-hydroxy-, ethyl ester (CA INDEX NAME)



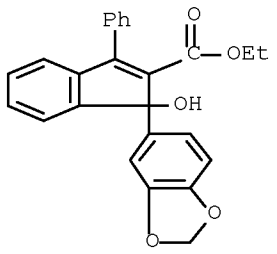
RN 150356-38-0 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 3-(1,3-benzodioxol-5-yl)-1-hydroxy-1-(3-methoxyphenyl)-, ethyl ester (CA INDEX NAME)



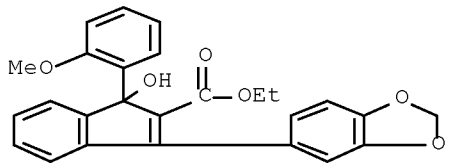
RN 150356-41-5 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1,3-bis(1,3-benzodioxol-5-yl)-1-hydroxy-, ethyl ester (CA INDEX NAME)



RN 150356-45-9 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-(1,3-benzodioxol-5-yl)-1-hydroxy-3-phenyl-, ethyl ester (CA INDEX NAME)

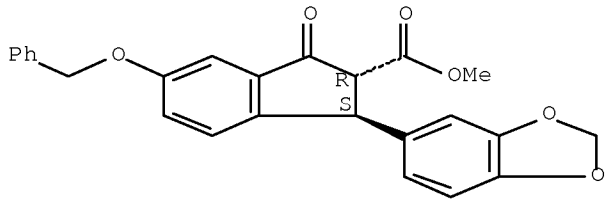


RN 150356-50-6 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 3-(1,3-benzodioxol-5-yl)-1-hydroxy-1-(2-methoxyphenyl)-, ethyl ester (CA INDEX NAME)

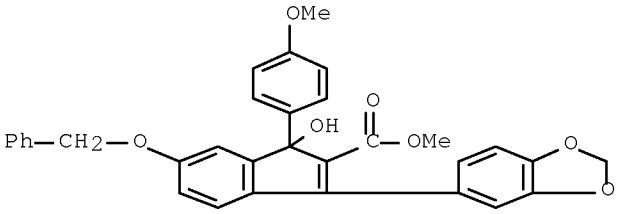


RN 150356-55-1 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-(1,3-benzodioxol-5-yl)-2,3-dihydro-3-oxo-5-(phenylmethoxy)-, methyl ester, (1R,2S)-rel- (CA INDEX NAME)

Relative stereochemistry.

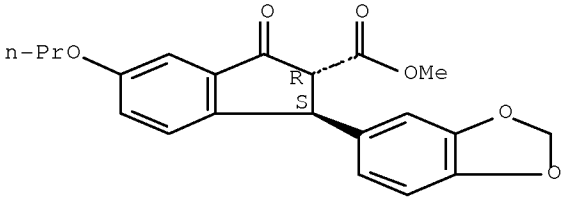


RN 150356-57-3 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 3-(1,3-benzodioxol-5-yl)-1-hydroxy-1-(4-methoxyphenyl)-6-(phenylmethoxy)-, methyl ester (CA INDEX NAME)

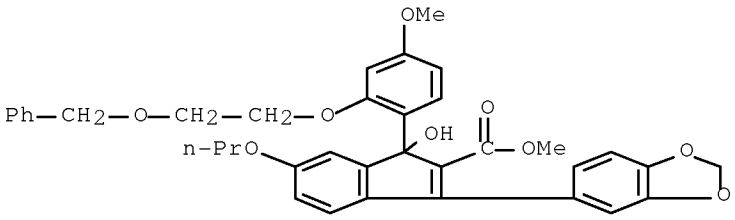


RN 150356-61-9 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-(1,3-benzodioxol-5-yl)-2,3-dihydro-3-oxo-5-propoxy-, methyl ester, (1R,2S)-rel- (CA INDEX NAME)

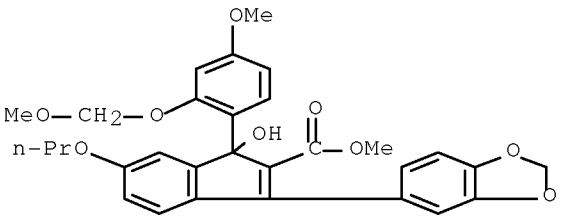
Relative stereochemistry.



RN 214271-73-5 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 3-(1,3-benzodioxol-5-yl)-1-hydroxy-1-[4-methoxy-2-[2-(phenylmethoxy)ethoxy]phenyl]-6-propoxy-, methyl ester (CA INDEX NAME)



IT 156023-59-5P
RL: PEP (Physical, engineering or chemical process); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)
(resolution; preparation of indanecarboxylic acid derivs. as endothelin receptor antagonists)
RN 156023-59-5 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 3-(1,3-benzodioxol-5-yl)-1-hydroxy-1-[4-methoxy-2-(methoxymethoxy)phenyl]-6-propoxy-, methyl ester (CA INDEX NAME)



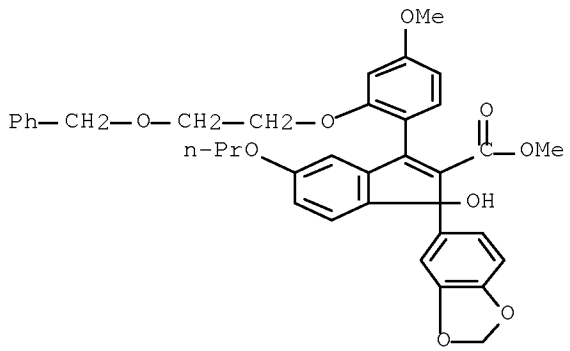
REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L106 ANSWER 22 OF 40 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1998:118608 ZCAPLUS Full-text
DOCUMENT NUMBER: 128:184694
ORIGINAL REFERENCE NO.: 128:36399a,36402a
TITLE: Endothelin receptor antagonists
INVENTOR(S): Elliott, John Duncan; Lago, Maria Amparo
PATENT ASSIGNEE(S): Smithkline Beecham Corp., USA
SOURCE: U.S., 10 pp., Cont.-in-part of U.S. Ser. No. 336,444.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 4
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5716985	A	19980210	US 1995-450938	19950523
CZ 287406	B6	20001115	CZ 1994-1109	19921029
ZA 9208467	A	19930505	ZA 1992-8467	19921103
ES 2062927	A1	19941216	ES 1992-2548	19921217
ES 2062927	B1	19950701		
US 5817693	A	19981006	US 1994-336444	19941109
PRIORITY APPLN. INFO.:			US 1991-787870 B2	19911105
			US 1992-854195 B2	19920320
			US 1993-66818 B2	19930427
			US 1994-336444 A2	19941109
			CS 1994-1109 A	19921029

OTHER SOURCE(S): MARPAT 128:184694
AB Novel indane and indene derivs. are described which are endothelin receptor antagonists. E.g., (1RS,2SR,3RS)-3-[2-(2-hydroxy-1-ethoxy)-4- methoxyphenyl]-1-(3,4-methylenedioxyphenyl)-5-(1-propoxy)indan-2- carboxylic acid was prepared A inhalant formulation was given.
IC ICM A61K031-36
ICS A61K031-44; A61K031-335; A61K031-19
INCL 514464000
CC 63-6 (Pharmaceuticals)
Section cross-reference(s): 1, 25
IT 1462-37-9P, 2-Benzyloxyethyl bromide 63604-94-4P 190969-68-7P
203396-16-1P 203396-17-2P 203396-18-3P 203396-19-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(indan derivs. as endothelin receptor antagonists)
IT 203396-16-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(indan derivs. as endothelin receptor antagonists)
RN 203396-16-1 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-(1,3-benzodioxol-5-yl)-1-hydroxy-3-[4-methoxy-2-[2-(phenylmethoxy)ethoxy]phenyl]-5-propoxy-, methyl ester (CA INDEX NAME)



L106 ANSWER 23 OF 40 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1997:796178 ZCAPLUS Full-text
DOCUMENT NUMBER: 128:108426
ORIGINAL REFERENCE NO.: 128:21129a,21132a
TITLE: Electrophotographic photoreceptor using novel charge-transporting agent
INVENTOR(S): Sanada, Hirofumi; Kinoshita, Akira; Shibata, Toyoko; Suzuki, Tomoko; Watanabe, Kazumasa; Hai, Genko
PATENT ASSIGNEE(S): Konica Co., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 49 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 09319110	A	19971212	JP 1996-132074	19960527

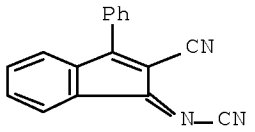
PRIORITY APPLN. INFO.: JP 1996-132074 19960527
OTHER SOURCE(S): MARPAT 128:108426
AB The photoreceptor contains novel specific heterocyclic or aromatic compds. described by 15 Markush structures as charge-transporting agents. The photoreceptor shows high photosensitivity, low residual potential, and durability in repeated use.
IC ICM G03G005-06
ICS G03G005-06
CC 74-3 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)
IT 641-57-6 3306-93-2 16917-81-0 17952-96-4 35491-56-6 51003-32-8 82873-06-1 99971-66-1 119014-16-3 119014-17-4 201355-67-1 201355-68-2 201355-69-3 201355-70-6 201355-71-7 201355-72-8 201355-73-9 201355-74-0 201355-75-1 201355-76-2 201355-77-3 201355-78-4 201355-81-9 201355-83-1 201355-85-3 201355-87-5 201355-89-7 201355-91-1 201355-93-3 201355-96-6 201356-00-5 201356-11-8 201356-14-1 201356-18-5 201356-21-0 201356-25-4

201356-28-7 201356-30-1 201356-33-4 201356-39-0 201356-41-4
201356-43-6 201356-46-9 201356-48-1 201356-49-2 201356-50-5
201356-51-6 201356-55-0 201356-57-2 201356-58-3 201356-59-4
201356-60-7 201356-61-8 201356-62-9 201356-64-1 201356-67-4
201356-71-0 201356-73-2 201356-77-6 201356-79-8 201356-81-2
201356-84-5 201356-87-8 201356-89-0 201356-90-3 201356-91-4
201356-93-6 201356-94-7 201356-96-9 201356-97-0 201356-99-2
201357-02-0 201357-03-1 201357-04-2 201357-06-4 201357-07-5
201357-09-7 201357-11-1 201357-12-2 201357-13-3 201357-15-5
201357-16-6 201357-17-7 201357-19-9 201357-21-3
RL: DEV (Device component use); USES (Uses)
(electrophotog. photoreceptor using novel charge-transporting agent)

IT 201355-67-1
RL: DEV (Device component use); USES (Uses)
(electrophotog. photoreceptor using novel charge-transporting agent)

RN 201355-67-1 ZCAPLUS

CN Cyanamide, (2-cyano-3-phenyl-1H-inden-1-ylidene)- (9CI) (CA INDEX NAME)



L106 ANSWER 24 OF 40 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1997:789557 ZCAPLUS Full-text

DOCUMENT NUMBER: 128:48026

ORIGINAL REFERENCE NO.: 128:9427a,9430a

TITLE: 1-oxo-3-Aryl-1H-indene-2-carboxylic acid derivatives as selective inhibitors of fibroblast growth factor receptor-1 tyrosine kinase

AUTHOR(S): Barvian, M. R.; Panek, R. L.; Lu, G. H.; Kraker, A. J.; Amar, A.; Hartl, B.; Hamby, J. M.; Showalter, H. D. H.

CORPORATE SOURCE: Parke-Davis Pharmaceutical Research, Division of Warner-Lambert Co., Ann Arbor, MI, 48105, USA

SOURCE: Bioorganic & Medicinal Chemistry Letters (1997), 7(22), 2903-2908
CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Fibroblast growth factor receptor (FGFr) mediated signal transduction is implicated in vascular proliferative diseases and some cancers. Thus, Me 1-oxo-3-phenyl-1H-indene-2-carboxylic ester was identified as a small mol. inhibitor of the tyrosine kinase activity of FGFr-1, (IC50 = 5.1 μM). The synthesis and structure-activity studies about this template core were reported. N example compound thus prepared was N-methyl-1-oxo-3- phenyl-1H-Indene-2-carboxamide. Addnl., screening of this series against a panel of tyrosine kinases shows selective inhibition of FGFr.

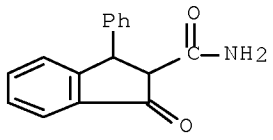
CC 25-23 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
Section cross-reference(s): 1

IT 4708-92-3 28858-00-6 200057-27-8 200057-29-0 200057-31-4
200057-32-5 200057-33-6 200057-35-8 200057-36-9 200057-38-1

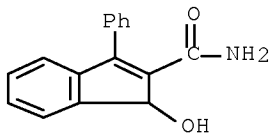
200057-40-5 200057-42-7 200057-43-8 200057-45-0
200057-46-1 200057-48-3
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(preparation of oxo(aryl)indenecarboxylic acid derivs. as inhibitor of fibroblast growth factor receptor tyrosine kinase)

IT 28858-00-6 200057-43-8
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(preparation of oxo(aryl)indenecarboxylic acid derivs. as inhibitor of fibroblast growth factor receptor tyrosine kinase)

RN 28858-00-6 ZCAPLUS
CN 1H-Indene-2-carboxamide, 2,3-dihydro-1-oxo-3-phenyl- (CA INDEX NAME)



RN 200057-43-8 ZCAPLUS
CN 1H-Indene-2-carboxamide, 1-hydroxy-3-phenyl- (CA INDEX NAME)



REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

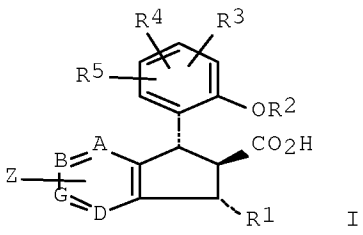
L106 ANSWER 25 OF 40 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1997:515322 ZCAPLUS Full-text
DOCUMENT NUMBER: 127:121712
ORIGINAL REFERENCE NO.: 127:23477a,23480a
TITLE: Stereoselective synthesis of endothelin receptor antagonists, particularly 1-(3,4-methylenedioxyphenyl)indane-2-carboxylic acids, using chiral auxiliaries such as carbohydrates.
INVENTOR(S): Mills, Robert John; Kowalski, Conrad John; Ping, Li-jen; Gombatz, Kerry Joseph
PATENT ASSIGNEE(S): Smithkline Beecham Corporation, USA; Mills, Robert John; Kowalski, Conrad John; Ping, Li-Jen; Gombatz, Kerry Joseph
SOURCE: PCT Int. Appl., 101 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9717071	A1	19970515	WO 1996-US18084	19961108
W: AL, AM, AU, BB, BG, BR, CA, CN, CZ, EE, GE, HU, IL, IS, JP, KG, KP, KR, LK, LR, LT, LV, MD, MG, MK, MN, MX, NO, NZ, PL, RO, SG, SI, SK, TR, TT, UA, US, UZ, VN, AZ, BY, KZ, RU, TJ, TM				
RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9676774	A	19970529	AU 1996-76774	19961108
EP 915699	A1	19990519	EP 1996-939654	19961108
R: BE, CH, DE, ES, FR, GB, IT, LI, NL				
JP 2000507918	T	20000627	JP 1997-518378	19961108
US 6080862	A	20000627	US 1998-68427	19980508
US 6162932	A	20001219	US 1999-296471	19990422

PRIORITY APPLN. INFO.:
US 1995-6348P P 19951108
US 1995-6347P P 19951108
WO 1996-US18084 W 19961108

OTHER SOURCE(S): CASREACT 127:121712; MARPAT 127:121712

GI



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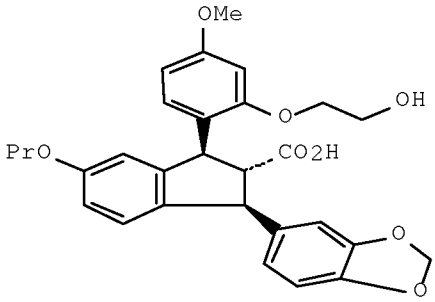


II

AB The invention is directed to a synthetic route for preparing endothelin receptor antagonists (no data) of formula I [R1 = (un)substituted 3,4-methylenedioxyphenyl; R2 = CH2CH2OH, (CH2)pCO2H; p = 1-3; R3, R4, R5 = H, alkyl, alkoxy, OH; A, B, G, D = CH; or 1 of them = N and others = CH; Z = H, OH, alkoxy, alkyl] and their enantiomers, as well as to chiral intermediates thereof. The route uses chiral auxiliaries to give I in enantiomerically or diastereomerically pure form, without the need to resort to chromatog. purification For example, title compound II was prepared in several steps. Reaction of 2,3:5,6-di-O-isopropylidene-α-D- mannofuranosyl chloride with 2-bromo-5-methoxyphenol gave a chiral glycoside, which underwent a chiral Grignard reaction with an indenone derivative to give an indenol product with an (R)/(S) diastereomer ratio of 88:12. The intermediate was purified by crystallization to a diastereomeric excess (de) of 99.5% in 69% yield. Subsequent hydrogenolysis of the indenol derivative, followed by epimerization, hydroxyethylation, and hydrolysis, gave II.

IC ICM A61K031-435
ICS A61K031-70; C07D221-04

CC 28-5 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 45

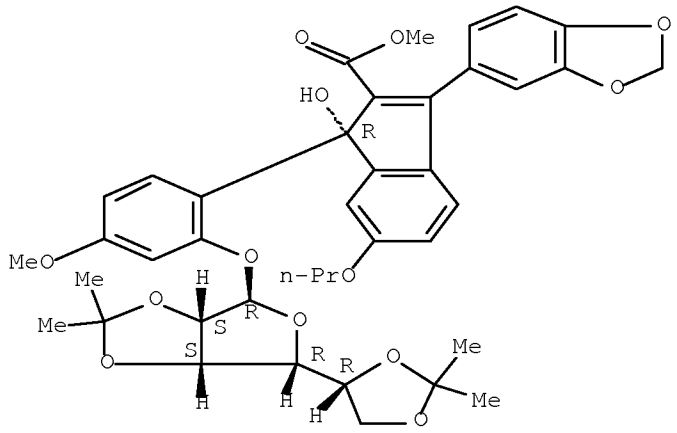
IT 192653-18-2P 192653-19-3P 192653-20-6P
RL: IMF (Industrial manufacture); PUR (Purification or recovery); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; stereoselective preparation of (methylenedioxyphenyl)indaneca
rboxylic acids as endothelin receptor antagonists)

IT 192653-18-2P 192653-19-3P
RL: IMF (Industrial manufacture); PUR (Purification or recovery); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; stereoselective preparation of (methylenedioxyphenyl)indaneca
rboxylic acids as endothelin receptor antagonists)

RN 192653-18-2 ZCAPLUS

CN 1H-Indene-2-carboxylic acid, 3-(1,3-benzodioxol-5-yl)-1-[2-[[2,3:5,6-bis-O-(1-methylethylidene)-α-D-mannofuranosyl]oxy]-4-methoxyphenyl]-1-hydroxy-6-propoxy-, methyl ester, (1R)- (CA INDEX NAME)

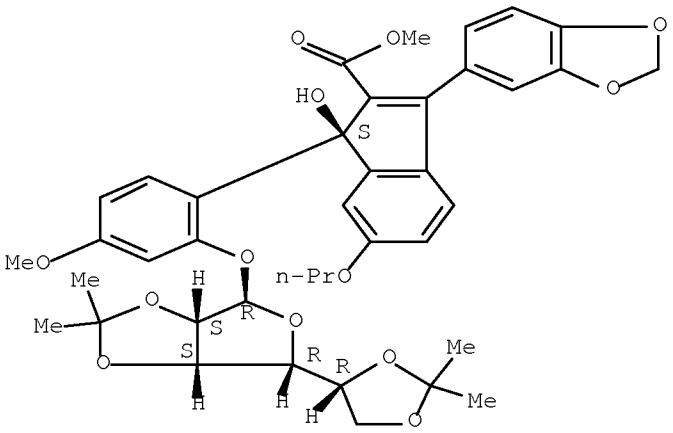
Absolute stereochemistry.



RN 192653-19-3 ZCAPLUS

CN 1H-Indene-2-carboxylic acid, 3-(1,3-benzodioxol-5-yl)-1-[2-[[2,3:5,6-bis-O-(1-methylethylidene)-α-D-mannofuranosyl]oxy]-4-methoxyphenyl]-1-hydroxy-6-propoxy-, methyl ester, (1S)- (CA INDEX NAME)

Absolute stereochemistry.



L106 ANSWER 26 OF 40 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1997:433648 ZCAPLUS Full-text
DOCUMENT NUMBER: 127:50628
ORIGINAL REFERENCE NO.: 127:9661a,9664a
TITLE: Preparation of 3-phenyl-1-piperonylindane-2-carboxylates and analogs
INVENTOR(S): Andemichael, Yemane Woldeselassie; Baine, Neil Howard; Clark, William Morrow; Kowalski, Conrad John; McGuire, Michael Anthony; Mills, Robert John
PATENT ASSIGNEE(S): Smithkline Beecham Corporation, USA
SOURCE: PCT Int. Appl., 98 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9717342	A1	19970515	WO 1996-US18846	19961108
W: AL, AM, AU, BB, BG, BR, CA, CN, CZ, EE, GE, HU, IL, IS, JP, KG, KP, KR, LK, LR, LT, LV, MD, MG, MK, MN, MX, NO, NZ, PL, RO, SG, SI, SK, TR, TT, UA, US, UZ, VN, AZ, BY, KZ, RU, TJ, TM				
RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
IN 1996DE02457	A	20050311	IN 1996-DE2457	19960711
CA 2236937	A1	19970515	CA 1996-2236937	19961108
AU 9710820	A	19970529	AU 1997-10820	19961108
AU 711450	B2	19991014		
ZA 9609408	A	19970610	ZA 1996-9408	19961108
EP 880518	A1	19981202	EP 1996-940864	19961108
EP 880518	B1	20030402		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI				
CN 1206415	A	19990127	CN 1996-199421	19961108
CN 1084742	B	20020515		
BR 9611540	A	19990302	BR 1996-11540	19961108
HU 9901985	A2	19990928	HU 1999-1985	19961108
JP 2000500444	T	20000118	JP 1997-518416	19961108

NZ 323790	A	20000228	NZ 1996-323790		19961108
AT 236151	T	20030415	AT 1996-940864		19961108
ES 2191121	T3	20030901	ES 1996-940864		19961108
IN 1996DE02469	A	20050311	IN 1996-DE2469		19961111
TW 466236	B	20011201	TW 1997-86100704		19970123
NO 9802090	A	19980707	NO 1998-2090		19980507
US 6147232	A	20001114	US 1998-68581		19980508
HK 1016588	A1	20040206	HK 1999-101514		19990412
US 6288247	B1	20010911	US 2000-521172		20000308
MX 2001PA06359	A	20011108	MX 2001-PA6359		20010620
US 20020087011	A1	20020704	US 2001-949577		20010910
US 6479659	B2	20021112			
PRIORITY APPLN. INFO.:			US 1995-6345P	P	19951108
			WO 1996-US18846	W	19961108
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			US 2000-521172	A3	20000308

OTHER SOURCE(S): CASREACT 127:50628; MARPAT 127:50628

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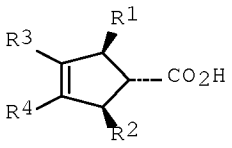


I

AB A multistep preparation for title compds. [I; R1 = ZOR5; R2 = (un)substituted piperonyl; R3R4 = CH:CHCH:CH, N:CHCH:CH, CH:NCH:CH, etc.; R5 = CH2CO2H or CH2CH2OH; Z = (un)substituted 1,2-phenylene] was given. Thus, (E)-PhCH2OZCOZ1CH:CHCOR [R = (S,S)-1,5-dimethyl-2-oxo-4-phenyl-3- imidazolyl, Z = 5-methoxy-1,2-phenylene, Z1 = 5-propoxy-1,2- phenylene](preparation given) was arylated/cyclized in a stereoselective Michael-type addition of piperonylmagnesium bromide and the product converted in several steps to, e.g., (+)-(1S, 2R, 3S)-3-[2-(2-hydroxyethyloxy)-4- methoxyphenyl]-3-(3, 4-methylenedioxyphenyl)-5-(propyloxy)indane-2- carboxylic acid.

IC ICM C07D405-08
ICS C07D317-60; C07D317-54; C07D317-52; C07D317-50; C07D233-38; C07D213-55; C07D213-54; C07D213-30; C07D213-26; C07C309-65; C07C305-26; C07C305-24; C07C063-10; C07C063-04; C07C049-317

CC 28-5 (Heterocyclic Compounds (More Than One Hetero Atom))

IT 92841-65-1P 139109-23-2P 167256-05-5P 190965-42-5P, 3-(1-Propyloxy)benzoic acid 190965-43-6P 190965-44-7P 190965-45-8P 190965-46-9P 190965-47-0P 190965-48-1P 190965-50-5P 190965-51-6P 190965-52-7P 191106-49-7P
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 3-phenyl-1-piperonylindane-2-carboxylates and analogs)

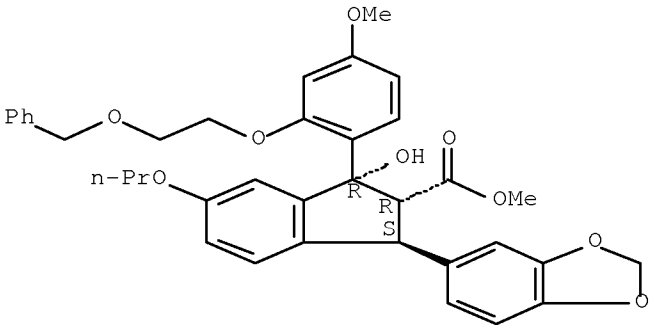
IT 190965-51-6P
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 3-phenyl-1-piperonylindane-2-carboxylates and analogs)

RN 190965-51-6 ZCAPLUS

CN 1H-Indene-2-carboxylic acid, 3-(1,3-benzodioxol-5-yl)-2,3-dihydro-1-hydroxy-1-[4-methoxy-2-[2-(phenylmethoxy)ethoxy]phenyl]-6-propoxy-, methyl

ester, [1R-(1α,2α,3β)]- (9CI) (CA INDEX NAME)

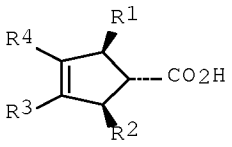
Absolute stereochemistry.



L106 ANSWER 27 OF 40 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1997:433634 ZCAPLUS Full-text
DOCUMENT NUMBER: 127:50627
ORIGINAL REFERENCE NO.: 127:9661a,9664a
TITLE: Preparation of 1-methylenedioxyphenyl-3-phenylindane-2-carboxylates and analogs
INVENTOR(S): Clark, William Morrow; Lantos, Ivan; Mills, Robert John; Pridgen, Robert John; Tickner, Ann Marie
PATENT ASSIGNEE(S): Smithkline Beecham Corporation, USA
SOURCE: PCT Int. Appl., 91 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 9717341	A1	19970515	WO 1996-US18465		19961108
W: AL, AM, AU, BB, BG, BR, CA, CN, CZ, EE, GE, HU, IL, IS, JP, KG, KP, KR, LK, LR, LT, LV, MD, MG, MK, MN, MX, NO, NZ, PL, RO, SG, SI, SK, TR, TT, UA, US, UZ, VN, AZ, BY, KZ, RU, TJ, TM					
RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG					
CA 2236926	A1	19970515	CA 1996-2236926		19961108
AU 9710542	A	19970529	AU 1997-10542		19961108
JP 2000500443	T	20000118	JP 1997-518411		19961108
EP 1019397	A1	20000719	EP 1996-941380		19961108
R: BE, CH, DE, ES, FR, GB, IT, LI, NL					
US 6143907	A	20001107	US 1997-776804		19970204
US 6355813	B1	20020312	US 2000-607173		20000629
PRIORITY APPLN. INFO.:			US 1995-6331P	P	19951108
			WO 1996-US18465	W	19961108
			US 1997-776804	A3	19970204

OTHER SOURCE(S): MARPAT 127:50627
GI



I

AB A multistep process for preparation of title compds. [I; R1 = ZR5; R2 = (un)substituted 3,4-methylenedioxyphenyl; R3R4 = CH:CHCH:CH, N:CHCH:CH, CH:NCH:CH, etc.; R5 = OCH2CO2H or OCH2CH2OH; Z = (un)substituted 1,2-phenylene] was given.

IC ICM C07D405-08
ICS C07D317-60; C07D317-54; C07D317-52; C07D317-50; C07D213-55; C07D213-54; C07D213-30; C07D213-26

CC 28-5 (Heterocyclic Compounds (More Than One Hetero Atom))

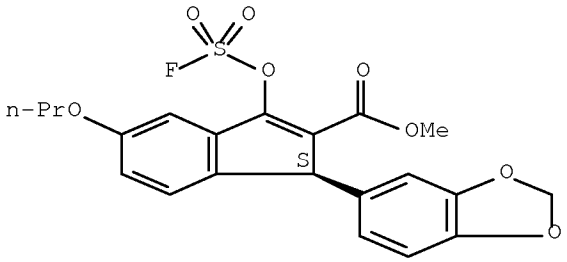
IT 150356-67-5P, 1-Bromo-4-methoxy-2-phenylmethoxybenzene 167256-05-5P 174527-88-9P 183474-19-3P, 4-Methoxy-2-phenylmethoxyphenylboronic acid 190965-48-1P 190965-52-7P 190965-53-8P 190969-63-2P 190969-64-3P 190969-65-4P 190969-66-5P 190969-67-6P 190969-68-7P, 1-Bromo-4-methoxy-2-(2-phenylmethoxyethoxy)benzene 190969-69-8P 191106-49-7P 191107-13-8P
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 1-methylenedioxyphenyl-3-phenylindane-2-carboxylates and analogs)

IT 190969-67-6P 191107-13-8P
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 1-methylenedioxyphenyl-3-phenylindane-2-carboxylates and analogs)

RN 190969-67-6 ZCAPLUS

CN 1H-Indene-2-carboxylic acid, 1-(1,3-benzodioxol-5-yl)-3-[(fluorosulfonyl)oxy]-5-propoxy-, methyl ester, (1S)- (CA INDEX NAME)

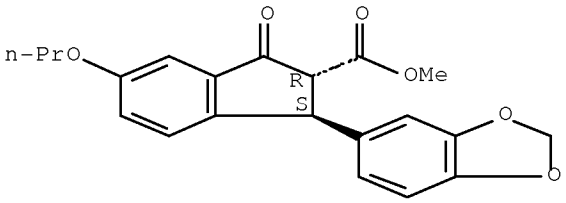
Absolute stereochemistry.



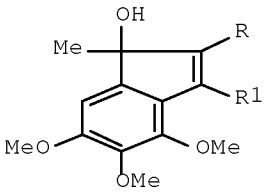
RN 191107-13-8 ZCAPLUS

CN 1H-Indene-2-carboxylic acid, 1-(1,3-benzodioxol-5-yl)-2,3-dihydro-3-oxo-5-propoxy-, methyl ester, (1S-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L106 ANSWER 28 OF 40 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1996:431646 ZCAPLUS Full-text
DOCUMENT NUMBER: 125:168304
ORIGINAL REFERENCE NO.: 125:31552h,31553a
TITLE: Palladium-Assisted Formation of Carbon-Carbon Bonds. 6. Study of the Reactivity of (o-Formylaryl)- or (o-Acetylaryl)palladium Complexes with Alkynes. Synthesis of Indenones and Indenols
AUTHOR(S): Vicente, Jose; Abad, Jose-Antonio; Gil-Rubio, Juan
CORPORATE SOURCE: Facultad de Quimica, Universidad de Murcia, Murcia, E-30071, Spain
SOURCE: Organometallics (1996), 15(16), 3509-3519
CODEN: ORGND7; ISSN: 0276-7333
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 125:168304
GI



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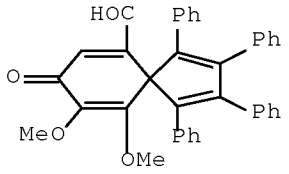


II

AB The reaction of (BzPh3P)2[Pd(R1)Cl(μ-Cl)]2 (1; Bz = PhCH2; R1 = 6-formyl-2,3,4-trimethoxyphenyl) with PhC.tplbond.CPh gives a 6.5:1 mixture of 4,5,6-trimethoxy-2,3-diphenylindenone (2) and 4,5,6-trimethoxy-2,3- diphenyl-1H-indenol (3). When the same reaction is carried out with MeO2CC.tplbond.CCO2Me or with Me3SiC.tplbond.CSiMe3, 4,5,6-trimethoxy-2,3-bis(methoxycarbonyl)indenone (4) and R1C.tplbond.CSiMe3 (5) were obtained, resp. The reactions of PhC.tplbond.CPh with [Pd(R1)Cl(bpy)] (6; bpy = 2,2'-bipyridine), in the presence of AgClO4, or with [Pd(R1)(MeCN)(bpy)]ClO4 (7) yield 3 and [Pd(μ-OH)(bpy)]2(ClO4)2 (8a). If 7 reacts with PhC.tplbond.CPh under anhydrous conditions, the indenone 2 was obtained. [Pd(R2)(MeCN)(bpy)]ClO4 (9; R2 = 2-formyl-3,4,5- trimethoxyphenyl) reacts with PhC.tplbond.CPh, giving 5,6,7-trimethoxy-2,3- diphenyl-1H-indenol (10) or, under anhydrous conditions, 5,6,7-trimethoxy-2,3- diphenylindenone (11). A 1:1 mixture of both compds. was obtained by reacting [Pd(η2-R2)(μ-Cl)]2 (12)

with PhC.tplbond.CPh. [Pd(η2-R3)(bpy)](CF3SO3) (13; R3 = 6-acetyl-2,3,4-trimethoxyphenyl) reacts with the alkynes RC.tplbond.CR' (R = R' = Ph, 4-tolyl, CO2Me, Me, Et; R = Ph, R' = CO2Et, 4-nitrophenyl, 4-methoxyphenyl, Me; R = tBu, R' = H, Me), yielding [Pd(μ-OH)(bpy)]2(CF3SO3)2 (8b) and 1-methylindenols I (sometimes mixed with regioisomer with R and R' reversed). The catalytic reaction of [Hg(R1)2] with PhC.tplbond.CPh and CuCl2 in the presence of Q2[Pd2Cl6] (1:6:2:0.05; Q = Me4N, PhCH2PPh3) gives the indenol 3 in 62% yield with respect to the group R present in the mercurial compound When a similar reaction (Q = PhCH2PPh3) is carried out under N2, the spirocyclic compound II.

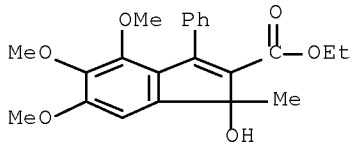
CC 29-13 (Organometallic and Organometalloidal Compounds)
Section cross-reference(s): 25

IT 144647-96-1P 144647-97-2P 144647-98-3P 180400-38-8P, 3,4,5-Trimethoxy-2-(2-trimethylsilylethynyl)benzaldehyde 180400-41-3P 180400-42-4P 180400-43-5P 180400-44-6P 180400-45-7P 180400-46-8P 180400-47-9P 180400-48-0P 180400-49-1P 180400-50-4P 180400-51-5P 180400-52-6P 180400-53-7P 180400-54-8P, 10-Formyl-6,7-dimethoxy-1,2,3,4-tetraphenylspiro[4.5]1,3,6,9-decatetraen-8-one 180400-55-9P 180400-56-0P 180400-57-1P 180400-58-2P 180400-59-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(palladium-assisted preparation)

IT 180400-48-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(palladium-assisted preparation)

RN 180400-48-0 ZCAPLUS

CN 1H-Indene-2-carboxylic acid, 1-hydroxy-4,5,6-trimethoxy-1-methyl-3-phenyl-, ethyl ester (CA INDEX NAME)



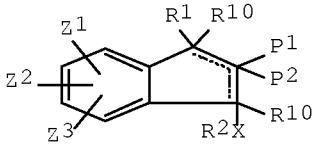
L106 ANSWER 29 OF 40 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1995:763506 ZCAPLUS Full-text
DOCUMENT NUMBER: 123:169596
ORIGINAL REFERENCE NO.: 123:30279a,30282a
TITLE: Preparation of indane- and indene-derivative endothelin receptor antagonists
INVENTOR(S): Cousins, Russell Donovan; Elliott, John Duncan; Lago, Maria Amparo; Leber, Jack Dale; Peishoff, Catherine Elizabeth
PATENT ASSIGNEE(S): SmithKline Beecham Corp., USA
SOURCE: PCT Int. Appl., 45 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 4
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

WO 9425013		A1	19941110	WO 1994-US4603	19940426
W: AU, BB, BG, BR, BY, CA, CN, CZ, FI, HU, JP, KP, KR, KZ, LK, MG, MN, MW, NO, NZ, PL, RO, RU, SD, SI, SK, UA, US					
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG					
CA 2160914		A1	19941110	CA 1994-2160914	19940426
AU 9467750		A	19941121	AU 1994-67750	19940426
AU 682038		B2	19970918		
BR 9406572		A	19960130	BR 1994-6572	19940426
EP 699069		A1	19960306	EP 1994-915903	19940426
EP 699069		B1	20020213		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE					
CN 1124923		A	19960619	CN 1994-192388	19940426
CN 1129428		B	20031203		
HU 73763		A2	19960930	HU 1995-1931	19940426
JP 08510211		T	19961029	JP 1994-524496	19940426
JP 3346571		B2	20021118		
PL 175392		B1	19981231	PL 1994-311272	19940426
RU 2130920		C1	19990527	RU 1995-122388	19940426
AT 213156		T	20020215	AT 1994-915903	19940426
PT 699069		T	20020731	PT 1994-915903	19940426
ES 2172535		T3	20021001	ES 1994-915903	19940426
CZ 291189		B6	20030115	CZ 1995-2835	19940426
US 6271399		B1	20010807	US 1995-459985	19950602
FI 9505103		A	19951026	FI 1995-5103	19951026
NO 9504291		A	19951221	NO 1995-4291	19951026
NO 313754		B1	20021125		
US 6087389		A	20000711	US 1998-99373	19980618
HK 1012252		A1	20030103	HK 1998-113510	19981215
US 6274737		B1	20010814	US 2000-574413	20000519
US 20020002177		A1	20020103	US 2001-901951	20010710
US 6448260		B2	20020910		
PRIORITY APPLN. INFO.:				US 1993-66818	A 19930427
				US 1991-787870	B2 19911105
				US 1992-854195	B2 19920320
				WO 1992-US9427	A2 19921029
				WO 1994-US4603	W 19940426
				US 1994-336444	A1 19941109
				US 1998-99373	A3 19980618
				US 2000-574413	A3 20000519
OTHER SOURCE(S):		MARPAT 123:169596			

GI



I

AB The title compds. [I; P1, P2 = (un)substituted alkyl, (un)substituted carboxyalkyl, etc.; R1 = (un)substituted arylalkyl, (un)substituted hyeterocyclylalkyl, (un)substituted cycloalkyl; R2 = H, (un)substituted aryl, C1-4 alkyl; R10 = H, OH, alkoxy, halogen, (un)substituted acylamino, etc; X = alkylene, O, (un)substituted NR6, S(O)q; R6 = H, alkyl; q = 0-2; Z1-Z3 = H, alkyl, alkenyl, alkynyl, OH, alkoxy, halogen, (un)substituted acylamino, etc.]

[e.g., (+)(1S,2R,3S)-3-(2-carboxymethoxy-4-methoxyphenyl)- 1-(3,4-methylenedioxyphenyl)-5-(prop-1-yloxy)indane-2-carboxylic acid; m.p. 99-102°], useful as endothelin receptor antagonists (no data), are prepared and I-containing formulations presented.

IC ICM A61K031-075
ICS A61K031-165; A61K031-185; A61K031-18; A61K031-19; A61K031-21; A61K031-335; A61K031-34; A61K031-35; A61K031-36; A61K031-365; C07C061-20; C07C062-32; C07C069-74; C07C309-25; C07C309-63; C07C311-14; C07D317-50

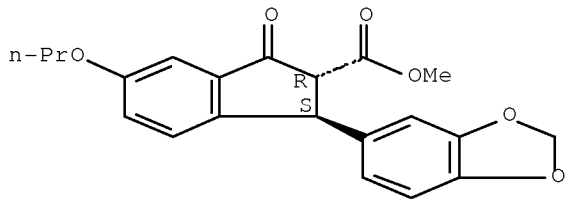
CC 28-5 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 25, 63

IT 63604-94-4P 121704-77-6P 133730-24-2P 150356-60-8P
150356-61-9P 150356-62-0P 156023-58-4P 156023-61-9P
156129-15-6P 167084-46-0P 167084-47-1P 167084-48-2P
167084-49-3P 167084-50-6P 167084-51-7P 167084-52-8P 167084-53-9P
167084-54-0P 167084-55-1P 167084-56-2P 167084-57-3P 167084-58-4P
167084-59-5P 167084-60-8P 167084-61-9P 167084-62-0P 167256-04-4P
167256-05-5P 167256-12-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of indane- and indene-derivative endothelin receptor antagonists)

IT 150356-61-9P 167084-46-0P 167084-47-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of indane- and indene-derivative endothelin receptor antagonists)

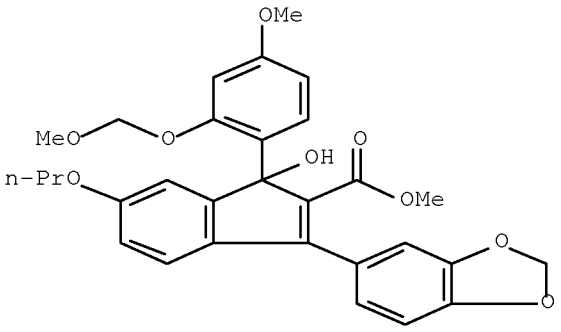
RN 150356-61-9 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-(1,3-benzodioxol-5-yl)-2,3-dihydro-3-oxo-5-propoxy-, methyl ester, (1R,2S)-rel- (CA INDEX NAME)

Relative stereochemistry.



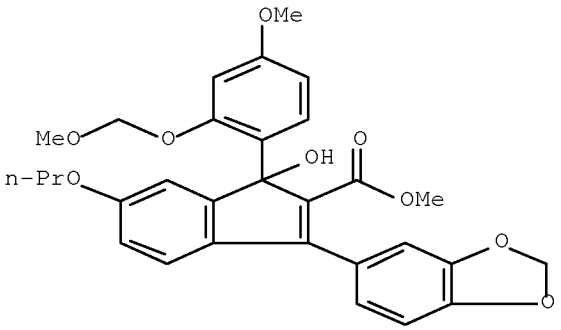
RN 167084-46-0 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 3-(1,3-benzodioxol-5-yl)-1-hydroxy-1-[4-methoxy-2-(methoxymethoxy)phenyl]-6-propoxy-, methyl ester, (+)- (CA INDEX NAME)

Rotation (+).

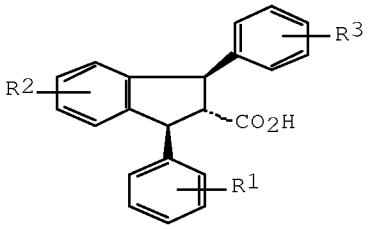


RN 167084-47-1 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 3-(1,3-benzodioxol-5-yl)-1-hydroxy-1-[4-methoxy-2-(methoxymethoxy)phenyl]-6-propoxy-, methyl ester, (-)- (CA INDEX NAME)

Rotation (-).



L106 ANSWER 30 OF 40 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1994:457097 ZCAPLUS Full-text
DOCUMENT NUMBER: 121:57097
ORIGINAL REFERENCE NO.: 121:10289a,10292a
TITLE: 1,3-Diarylindan-2-carboxylic Acids, Potent and Selective Non-Peptide Endothelin Receptor Antagonists
AUTHOR(S): Elliott, John D.; Lago, M. Amparo; Cousins, Russell D.; Gao, Aiming; Leber, Jack D.; Erhard, Karl F.; Nambi, Ponnal; Elshourbagy, Nabil A.; Kumar, Chandrika; et al.
CORPORATE SOURCE: Research and Development Division, SmithKline Beecham Pharmaceuticals, King of Prussia, PA, 19406-0939, USA
SOURCE: Journal of Medicinal Chemistry (1994), 37(11), 1553-7
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

AB A potent and specific ETA/ETB receptor antagonist, indanecarboxylic acid I [R1 = 3,4-OCH2O, R2 = 5-OPr, R3 = 2-HO2CCH2O, R4 = 4-OMe, II] (SB 209670) has been designed using 1H NMR derived conformational models of ET-1. Analogs I [R1 = H, 4-OMe; R2 = H, 5-OH, 5-OPr; R3 = H, 4-OMe, 3,4-OCH2O] were also prepared II is a competitive antagonist at both human ETA and ETB receptor sub-types with Ki values of 0.43 ± 0.09 nM and 14.7 ± 3 nM, resp.

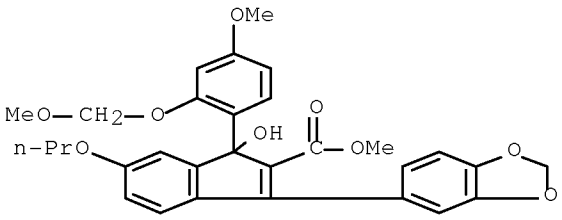
CC 25-23 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
Section cross-reference(s): 1

IT 150356-60-8P 150356-62-0P 156023-58-4P 156023-59-5P
156023-60-8P 156129-15-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, in preparation of diarylindancarboxylate)

IT 156023-59-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, in preparation of diarylindancarboxylate)

RN 156023-59-5 ZCAPLUS

CN 1H-Indene-2-carboxylic acid, 3-(1,3-benzodioxol-5-yl)-1-hydroxy-1-[4-methoxy-2-(methoxymethoxy)phenyl]-6-propoxy-, methyl ester (CA INDEX NAME)



L106 ANSWER 31 OF 40 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1994:106563 ZCAPLUS Full-text
DOCUMENT NUMBER: 120:106563
ORIGINAL REFERENCE NO.: 120:18781a,18784a
TITLE: Indane derivatives and their use as endothelin receptor antagonists
INVENTOR(S): Cousins, Russell Donovan; Elliott, John Duncan; Lago, Maria Amparo; Leber, Jack Dale; Peishoff, Catherine Elisabeth
PATENT ASSIGNEE(S): SmithKline Beecham Corp., USA
SOURCE: PCT Int. Appl., 86 pp.

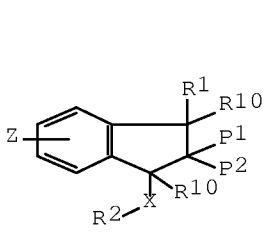
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 4
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9308799	A1	19930513	WO 1992-US9427	19921029
W: AT, AU, BB, BG, BR, CA, CH, CS, DE, DK, ES, FI, GB, HU, JP, KP, KR, LK, LU, MG, MN, MW, NL, NO, PL, RO, RU, SD, SE, UA, US				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, SN, TD, TG				
AU 9331259	A	19930607	AU 1993-31259	19921029
AU 669866	B2	19960627		
EP 612244	A1	19940831	EP 1992-925061	19921029
EP 612244	B1	20010919		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, SE				
HU 67665	A2	19950428	HU 1994-1319	19921029
BR 9206722	A	19950718	BR 1992-6722	19921029
RU 2125980	C1	19990210	RU 1994-27696	19921029
PL 176250	B1	19990531	PL 1992-303507	19921029
CZ 287406	B6	20001115	CZ 1994-1109	19921029
AT 205711	T	20011015	AT 1992-925061	19921029
SK 282098	B6	20011106	SK 1994-521	19921029
ES 2164054	T3	20020216	ES 1992-925061	19921029
RO 117847	B1	20020830	RO 1994-750	19921029
ZA 9208467	A	19930505	ZA 1992-8467	19921103
CN 1073161	A	19930616	CN 1992-114447	19921105
CN 1034569	B	19970416		
ES 2062927	A1	19941216	ES 1992-2548	19921217
ES 2062927	B1	19950701		
NO 9401650	A	19940701	NO 1994-1650	19940504
FI 9402059	A	19940704	FI 1994-2059	19940504
US 6271399	B1	20010807	US 1995-459985	19950602
CN 1145223	A	19970319	CN 1996-101622	19960110
US 6087389	A	20000711	US 1998-99373	19980618
HK 1012251	A1	20020419	HK 1998-113509	19981215
US 6274737	B1	20010814	US 2000-574413	20000519
US 20020002177	A1	20020103	US 2001-901951	20010710
US 6448260	B2	20020910		

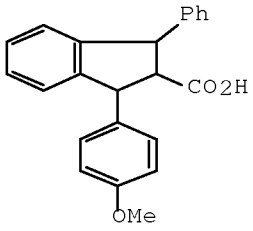
PRIORITY APPLN. INFO.:

US 1991-787870	A2	19911105
US 1992-854195	A2	19920320
CS 1994-1109	A	19921029
WO 1992-US9427	A	19921029
US 1993-66818	B2	19930427
WO 1994-US4603	A2	19940426
US 1994-336444	A1	19941109
US 1998-99373	A3	19980618
US 2000-574413	A3	20000519

OTHER SOURCE(S): MARPAT 120:106563
GI



I



II

AB The title compds. I (R1 = alkylaryl, etc.; R2 = H, aryl; R10 = alkylaryl, aryl, etc.; P1, R2 = substituted alkyl; Z = H, alkyl, etc.) and their use as endothelin receptor antagonists are claimed. I are useful as antihypertensives, treatment of renal failure or cerebrovascular disease. Addition reaction of 4-methoxyphenylmagnesium bromide with Et 1-oxo-3-phenylindene-2-carboxylate gave 1-(4-methoxyphenyl)-3-phenyl-2-indanecarboxylic acid (II). Data for the pharmacol. activity of I were not reported.

IC ICM A61K031-19
ICS A61K031-36; A61K031-41; A61K031-66; C07C061-20; C07C062-32; C07D257-04; C07D317-50; C07D405-08; C07F009-30; C07F009-38

CC 25-23 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
Section cross-reference(s): 1

ST indanecarboxylate prepn antihypertensive renal failure; cerebrovascular disease indanecarboxylate prepn; endothelin receptor antagonist indanecarboxylate prepn

IT Antihypertensives
(indanecarboxylate derivs. (endothelin receptor antagonists))

IT 34068-01-4P 63604-94-4P 81729-00-2P 121704-77-6P
150356-18-6P 150356-19-7P 150356-20-0P 150356-22-2P
150356-23-3P 150356-24-4P 150356-25-5P 150356-26-6P
150356-27-7P 150356-28-8P 150356-29-9P 150356-30-2P 150356-31-3P
150356-32-4P 150356-33-5P 150356-34-6P 150356-35-7P
150356-36-8P 150356-37-9P 150356-38-0P 150356-39-1P
150356-40-4P 150356-41-5P 150356-42-6P 150356-43-7P
150356-44-8P 150356-45-9P 150356-46-0P 150356-47-1P
150356-48-2P 150356-49-3P 150356-50-6P 150356-51-7P
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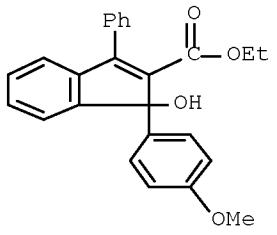
150356-60-8P 150356-61-9P 150356-62-0P 150356-63-1P
150356-64-2P 150356-65-3P 150356-66-4P 150356-67-5P 150356-68-6P
150356-71-1P 150356-72-2P 150356-73-3P 150356-74-4P 150356-75-5P
150356-76-6P 150356-77-7P 150356-78-8P 150356-79-9P 150356-80-2P
150356-81-3P 150356-82-4P 150356-83-5P 150356-84-6P 150356-85-7P
150408-20-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as intermediate for indanecarboxylic acid (endothelin receptor antagonist))

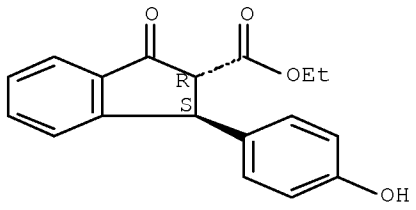
IT 150356-18-6P 150356-22-2P 150356-23-3P
150356-25-5P 150356-33-5P 150356-36-8P
150356-38-0P 150356-41-5P 150356-45-9P
150356-50-6P 150356-55-1P 150356-57-3P
150356-61-9P 150356-63-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as intermediate for indanecarboxylic acid (endothelin receptor antagonist))

RN 150356-18-6 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-hydroxy-1-(4-methoxyphenyl)-3-phenyl-, ethyl ester (CA INDEX NAME)



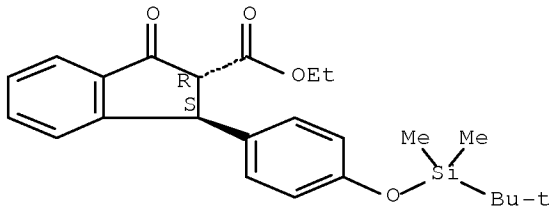
RN 150356-22-2 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 2,3-dihydro-1-(4-hydroxyphenyl)-3-oxo-, ethyl ester, (1R,2S)-rel- (CA INDEX NAME)

Relative stereochemistry.

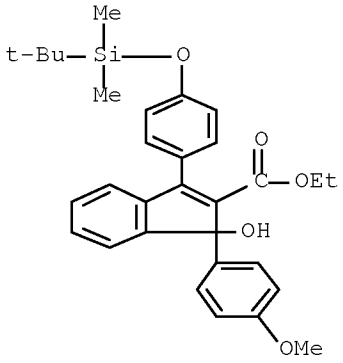


RN 150356-23-3 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-[4-[[(1,1-dimethylethyl)dimethylsilyl]oxy]phenyl]-2,3-dihydro-3-oxo-, ethyl ester, (1R,2S)-rel- (CA INDEX NAME)

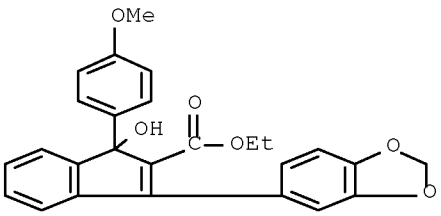
Relative stereochemistry.



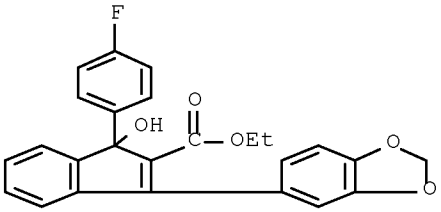
RN 150356-25-5 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 3-[4-[[(1,1-dimethylethyl)dimethylsilyl]oxy]phenyl]-1-hydroxy-1-(4-methoxyphenyl)-, ethyl ester (CA INDEX NAME)



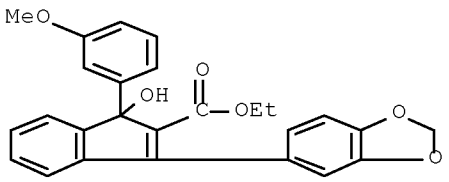
RN 150356-33-5 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 3-(1,3-benzodioxol-5-yl)-1-hydroxy-1-(4-methoxyphenyl)-, ethyl ester (CA INDEX NAME)



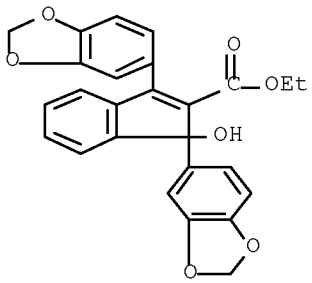
RN 150356-36-8 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 3-(1,3-benzodioxol-5-yl)-1-(4-fluorophenyl)-1-hydroxy-, ethyl ester (CA INDEX NAME)



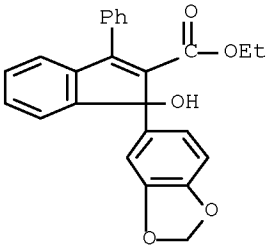
RN 150356-38-0 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 3-(1,3-benzodioxol-5-yl)-1-hydroxy-1-(3-methoxyphenyl)-, ethyl ester (CA INDEX NAME)



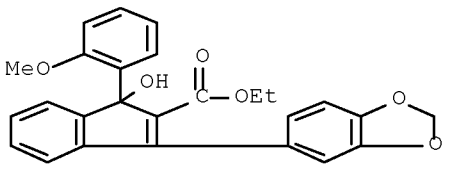
RN 150356-41-5 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1,3-bis(1,3-benzodioxol-5-yl)-1-hydroxy-, ethyl ester (CA INDEX NAME)



RN 150356-45-9 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-(1,3-benzodioxol-5-yl)-1-hydroxy-3-phenyl-, ethyl ester (CA INDEX NAME)

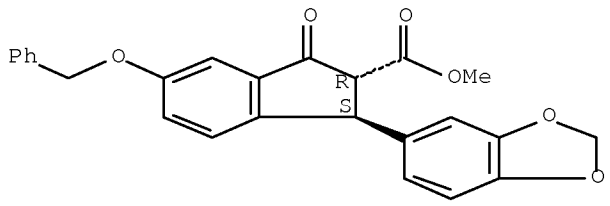


RN 150356-50-6 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 3-(1,3-benzodioxol-5-yl)-1-hydroxy-1-(2-methoxyphenyl)-, ethyl ester (CA INDEX NAME)

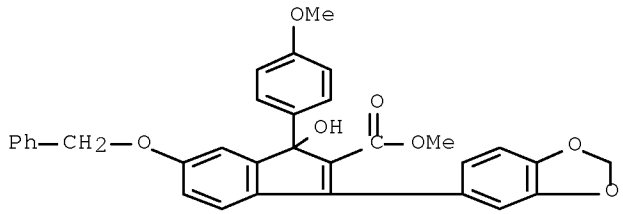


RN 150356-55-1 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-(1,3-benzodioxol-5-yl)-2,3-dihydro-3-oxo-5-(phenylmethoxy)-, methyl ester, (1R,2S)-rel- (CA INDEX NAME)

Relative stereochemistry.

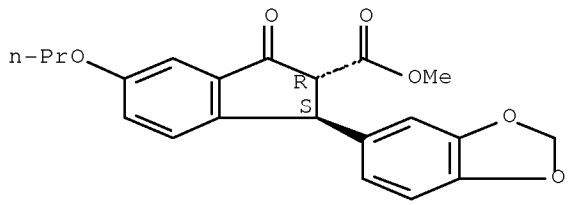


RN 150356-57-3 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 3-(1,3-benzodioxol-5-yl)-1-hydroxy-1-(4-methoxyphenyl)-6-(phenylmethoxy)-, methyl ester (CA INDEX NAME)

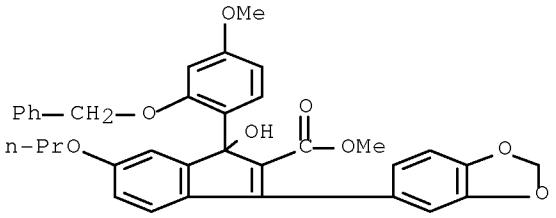


RN 150356-61-9 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-(1,3-benzodioxol-5-yl)-2,3-dihydro-3-oxo-5-propoxy-, methyl ester, (1R,2S)-rel- (CA INDEX NAME)

Relative stereochemistry.



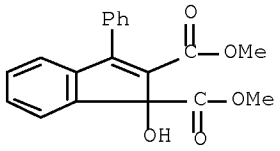
RN 150356-63-1 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 3-(1,3-benzodioxol-5-yl)-1-hydroxy-1-[4-methoxy-2-(phenylmethoxy)phenyl]-6-propoxy-, methyl ester (CA INDEX NAME)



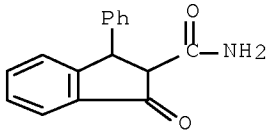
L106 ANSWER 32 OF 40 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1977:551372 ZCAPLUS Full-text
DOCUMENT NUMBER: 87:151372
ORIGINAL REFERENCE NO.: 87:23935a,23938a
TITLE: Photochemistry of 1,4-diphenyl-1,4-epoxy-1,4-dihydronaphthalene-2-carboxylate and -2,3-dicarboxylate esters
AUTHOR(S): Matheson, R. A. F.; McCulloch, A. W.; McInnes, A. G.; Smith, D. G.
CORPORATE SOURCE: Atl. Reg. Lab., Natl. Res. Counc. Canada, Halifax, NS, Can.
SOURCE: Canadian Journal of Chemistry (1977), 55(8), 1422-32
CODEN: CJCHAG; ISSN: 0008-4042
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Direct irradiation (2537 Å) of Me 1,4-diphenyl-1,4-epoxy-1,4-dihydronaphthalene-2-carboxylate (I) affords Me 2,4-diphenyl-3-benzoxepine- 1-carboxylate and Me 1-benzoyl-3-phenylindene-2-carboxylate (II), while acetone-sensitized irradiation yields mainly II. Direct irradiation of dimethyl 1,4-diphenyl-1,4-epoxy-1,4-dihydronaphthalene-2,3-dicarboxylate (III) affords a mixture of dimethyl 2,4-diphenyl-3-benzoxepine-1,5-dicarboxylate, dimethyl 1-benzoyl-3-phenylindene-1,2-dicarboxylate (IV), and dimethyl 1-benzoyl-2-phenylindene-1,3-dicarboxylate. Sensitized irradiation yields mainly IV. The formation of II and IV as major products of photorearrangement of I and III is consistent with a di-π-methane pathway. The AlCl3-catalyzed rearrangement of III yields a mixture of dimethyl 2,4-diphenyl-1(2H)-naphthalenone-2,3-dicarboxylate and Me 1,3-diphenyl-4-hydroxynaphthalene-2-carboxylate V, while that of I affords only V.

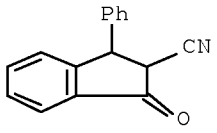
CC 22-4 (Physical Organic Chemistry)
IT 55302-51-7P 64362-20-5P 64362-21-6P 64362-22-7P 64362-24-9P
64362-25-0P 64362-26-1P 64362-27-2P 64362-28-3P 64362-29-4P
64362-30-7P 64362-31-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
IT 64362-30-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 64362-30-7 ZCAPLUS
CN 1H-Indene-1,2-dicarboxylic acid, 1-hydroxy-3-phenyl-, dimethyl ester (9CI) (CA INDEX NAME)



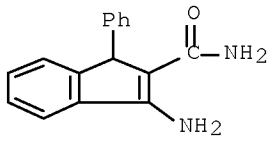
L106 ANSWER 33 OF 40 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1970:487880 ZCAPLUS Full-text
DOCUMENT NUMBER: 73:87880
ORIGINAL REFERENCE NO.: 73:14365a,14368a
TITLE: Substituted 5H-indeno[1,2-d-pyrimidines
AUTHOR(S): Campaigne, Ernest; Burton, Harold R.
CORPORATE SOURCE: Chem. Lab., Indiana Univ., Bloomington, IN, USA
SOURCE: Journal of Heterocyclic Chemistry (1970), 7(4), 937-40
CODEN: JHTCAD; ISSN: 0022-152X
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB 4-Chloro-5-phenylindeno[1,2-d]pyrimidine (I) is treated with alkylamines and dialkylamines to give the corresponding 4-amino derivs. (II). I is prepared from 2-carbamoyl-3-phenylindanone (III) via 5-phenyl-3H-indeno[1,2-d]pyrimidin-4-one.
CC 28 (Heterocyclic Compounds (More Than One Hetero Atom))
IT 245-02-3DP, 5H-Indeno[1,2-d]pyrimidine, derivs. 3713-63-1DP, 1H-Indeno[1,2-d]pyrimidine, derivs. 28857-98-9P 28857-99-0P 28858-00-6P 28858-01-7P 28858-02-8P 28858-03-9P 28858-04-0P 28858-05-1P 28858-06-2P 28858-08-4P 28858-09-5P 28858-10-8P 28858-11-9P 28858-12-0P 28858-13-1P 28858-14-2P 28858-15-3P 29878-24-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
IT 28858-00-6P 28858-01-7P 28858-03-9P 28858-04-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 28858-00-6 ZCAPLUS
CN 1H-Indene-2-carboxamide, 2,3-dihydro-1-oxo-3-phenyl- (CA INDEX NAME)



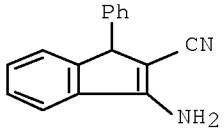
RN 28858-01-7 ZCAPLUS
CN 2-Indancarbonitrile, 1-oxo-3-phenyl- (6CI, 8CI) (CA INDEX NAME)



RN 28858-03-9 ZCAPLUS
CN Indene-2-carboxamide, 3-amino-1-phenyl- (8CI) (CA INDEX NAME)

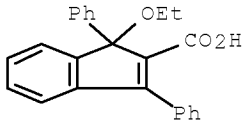


RN 28858-04-0 ZCAPLUS
CN Indene-2-carbonitrile, 3-amino-1-phenyl- (8CI) (CA INDEX NAME)



L106 ANSWER 34 OF 40 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1970:55551 ZCAPLUS Full-text
DOCUMENT NUMBER: 72:55551
ORIGINAL REFERENCE NO.: 72:10185a
TITLE: Grignard reagent containing a β-ether function
AUTHOR(S): Ficini, Jacqueline; Depezay, Jean C.
CORPORATE SOURCE: Lab. Chim. Org. Synthese, Paris, Fr.
SOURCE: Tetrahedron Letters (1969), (54), 4795-6
CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE: Journal
LANGUAGE: French
GI For diagram(s), see printed CA Issue.
AB The Greignard (Ia) of I is prepared and its reactions are studied. I is treated with Mg and hydrolyzed (H3O+) to give 80% II, m. 78°. The Ia is treated with CO2 and hydrolyzed to give 70% III, m. 172°.
CC 29 (Organometallic and Organometalloidal Compounds)
IT 25132-50-7P 25132-51-8P 25132-52-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
IT 25132-51-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 25132-51-8 ZCAPLUS
CN Indene-2-carboxylic acid, 1-ethoxy-1,3-diphenyl- (8CI) (CA INDEX NAME)



L106 ANSWER 35 OF 40 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1961:118391 ZCAPLUS Full-text
DOCUMENT NUMBER: 55:118391
ORIGINAL REFERENCE NO.: 55:22252i,22253a-g
TITLE: The reactions of 2-cyano-3-phenylindone with alkali
AUTHOR(S): Marsili, Antonio
CORPORATE SOURCE: Univ. Pisa, Italy
SOURCE: Annali di Chimica (Rome, Italy) (1961), 51, 237-51
CODEN: ANCRAI; ISSN: 0003-4592
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB Ethyl α-cyano-β-phenylcinnamate (9.4 g.) and 5 g. KOH in 10 ml. 50% EtOH was stirred 5 min., 10 ml. 50% EtOH added, and stirring continued 15 min. Then 200 ml. H2O was added, the undissolved portion filtered off, and the solution acidified to give 6.5 g. α-cyano-β-phenylcinnamic acid (I), m. 207-9°. I (12.4 g.) in 70 ml. concentrated H2SO4 was kept 3 hrs. and poured into ice with stirring to give 9.7 g. 2-cyano-3- phenylindone (II), m. 172-3.5°. II (0.5 g.), 0.5 g. NH2OH.HCl in 5 ml. absolute EtOH, and 5 ml. anhydrous C5H5N was warmed on the water bath 30 min. and diluted with H2O to give 0.5 g. oxime of II, m. 208-11° (MeOH); 2,4-dinitrophenylhydrazone of II m. 255-8° (AcOEt). II treated with KMnO4 in 10% Na2CO3 gave o-benzoylbenzoic acid, m. 127-9°. II (0.2 g.), 0.1 g. NaCl, 10 ml. 1:1 AcOH-concentrated H2SO4 warmed 3 hrs. on the water bath and poured into H2O gave 2-carbamoyl-3-phenylindone (III), m. 184-6°. III (0.5 g.) was refluxed in 10 ml. 15% KOH and cooled to give III K salt. To 1 g. II in 10 ml. 3% methanolic KOH, 0.2 g. NaBH4 was added with stirring and the mixture kept 20 hrs. to give 0.95 g. 2-cyano-3-phenylindan-1-one (IV), m. 147-50° (MeOH); 2,4-dinitrophenylhydrazone m. 201-3° (AcOEt-EtOH). Alternatively, 1 g. powdered II was hydrogenated at room temperature and 1 atmospheric in 35 ml. EtOH in the presence of 0.25 g. 5% PdAl2O3, the crystalline product (0.9 g.) dissolved in 15 ml. 20% alc. KOH, diluted with water, extracted with Et2O, and the aqueous phase acidified with dilute H2SO4 to give IV. Catalytic hydrogenation of II in alkaline medium failed. II (1 g.) refluxed 30 min. with 10% alc. KOH, diluted with water, acidified with concentrated HCl, the precipitate treated with 25 ml. 10% Na2CO3, filtered, and the solution treated with dilute HCl gave 0.45 g. β-(o-carboxyphenyl)cinnamonitrile (V), m. 189-92° (AcOH). II (0.5 g.) refluxed 4 hrs. in 7 ml. 20% aqueous KOH, cooled, acidified with concentrated HCl below 30°, and the precipitate washed with hot C6H6 gave β-(o-carboxyphenyl)cinnamic acid (VI), m. 176-81°. Alternatively, VI was prepared from III (yield 93%) and from V (93%). VI (0.2 g.) in 5 ml. quinoline was refluxed 10 min. in the presence of Cu powder, the mixture cooled, treated with concentrated HCl, extracted with Et2O, and the aqueous phase treated with dilute H2SO4 to give 0.06 g. o-(α- phenylvinyl)benzoic acid (VII), m. 134-6° (AcOH). VI (0.2 g.) heated in a microsublimator at 200°/2 mm., dissolved in 20 ml. 10% Na2CO3, extracted with Et2O and the aqueous phase treated with dilute H2SO4 gave 0.15

g. (3-phenylphthalidyl)acetic acid (VIII), m. 179-81° (aqueous AcOH). VI (0.1 g.) was heated at 200° until gas evolution ceased, the residue taken up with Et2O, extracted with 10% Na2CO3 and the organic phase distilled to give 0.02 g. 3-phenyl-3-methylphthalide (IX), m. 78-80°. Alternatively, IX was obtained by heating VII with concentrated H2SO4. VI (0.5 g.) in 10 ml. concentrated H2SO4 kept 40 min. gave 0.15 g. 2-carboxy-3- phenylindone, m. 159-61.5° (aqueous AcOH). V (0.5 g.) dissolved in 10 ml. concentrated H2SO4 and the mixture kept 40 min. gave 0.15 g. 9-cyanomethylanthrone (X), m. 192-3° (MeOH). X (0.1 g.) in 20 ml. Me2CO treated with Me2CO saturated with KMnO4, refluxed until the solution became colorless and filtered when hot, and the filtrate concentrated gave 0.06 g. anthraquinone. Ultraviolet spectra were given. 20 references.

CC 10F (Organic Chemistry: Condensed Carbocyclic Compounds)

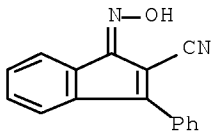
IT 874-35-1 7344-14-1 19744-64-0 100402-10-6 101278-69-7 111439-41-9
(Derived from data in the 6th Collective Formula Index (1957-1961))

IT 85-52-9P, Benzoic acid, o-benzoyl- 3048-65-5P, Indene, 3a,4,7,7a-tetrahydro- 10380-41-3P, Acrylic acid, 2-cyano-3,3-diphenyl- 17582-84-2P, Benzoic acid, o-(1-phenylvinyl)- 18019-56-2P, Phthalide, 3-methyl-3-phenyl- 21745-70-0P, Δ9(10H),α-Anthraceneacetonitrile, 10-oxo- 28858-01-7P, 2-Indancarbonitrile, 1-oxo-3-phenyl- 66528-17-4P, Indene-2-carboxylic acid, 1-oxo-3-phenyl- 94064-79-6P, Indene-2-carboxamide, 1-oxo-3-phenyl-, potassium derivative 101278-30-2P, Cinnamic acid, o-carboxy-β-phenyl- 101278-36-8P, 1-Phthalanacetic acid, 3-oxo-1-phenyl- 101727-23-5P, Benzoic acid, o-(2-cyano-1-phenylvinyl)- 102662-63-5P, 2-Indancarbonitrile, 1-oxo-3-phenyl-, (2,4-dinitrophenyl)hydrazone 102664-40-4P, Indone, 2-diphenylmethyl-3-ethylamino-
RL: PREP (Preparation)
(preparation of)

IT 101278-69-7 111439-41-9
(Derived from data in the 6th Collective Formula Index (1957-1961))

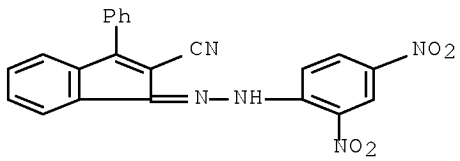
RN 101278-69-7 ZCAPLUS

CN Indene-2-carbonitrile, 1-oxo-3-phenyl-, oxime (6CI) (CA INDEX NAME)

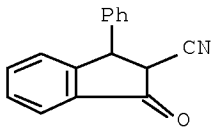


RN 111439-41-9 ZCAPLUS

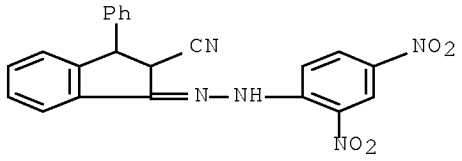
CN Indene-2-carbonitrile, 1-oxo-3-phenyl-, (2,4-dinitrophenyl)hydrazone (6CI) (CA INDEX NAME)



IT 28858-01-7P, 2-Indancarbonitrile, 1-oxo-3-phenyl-
102662-63-5P, 2-Indancarbonitrile, 1-oxo-3-phenyl-,
(2,4-dinitrophenyl)hydrazone
RL: PREP (Preparation)
(preparation of)
RN 28858-01-7 ZCAPLUS
CN 2-Indancarbonitrile, 1-oxo-3-phenyl- (6CI, 8CI) (CA INDEX NAME)

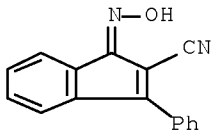


RN 102662-63-5 ZCAPLUS
CN 2-Indancarbonitrile, 1-oxo-3-phenyl-, (2,4-dinitrophenyl)hydrazone (6CI)
(CA INDEX NAME)

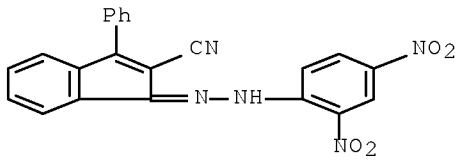


L106 ANSWER 36 OF 40 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1961:118390 ZCAPLUS Full-text
DOCUMENT NUMBER: 55:118390
ORIGINAL REFERENCE NO.: 55:22252g-i
TITLE: Synthesis of 2-benzhydryl-1,3-indandione and its 2-amino derivatives
AUTHOR(S): Arens, A.; Vanags, G.
CORPORATE SOURCE: Polytech. Inst., Riga
SOURCE: Zhurnal Obshchei Khimii (1961), 31, 117-23
CODEN: ZOKHA4; ISSN: 0044-460X
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB cf. CA 52, 2868b. Refluxing 2-nitro-2-benzhydryl-1,3-indandione with Na2S2O4 in EtOH 5 hrs., concentrating the mixture, and acidifying gave 74-8% 2-benzhydryl-1,3-indandione (I), m. 127-9°, which with Br in AcOH gave 2-bromo derivative (II), m. 147-8°. II and piperidine in Et2O-dioxane in 2 days gave 34.2% orange-yellow I piperidine salt, m. 202°, and 31.6% yellow 2-diphenylmethylene-1,3-indandione (III), m. 165-7°. II and Et2NH similarly gave red-orange I.Et2NH, decomposing 181-3°, and I. II and EtNH2 gave N-ethylimine analog of I, m. 164°. II and NH3 in dioxane gave in 2 hrs. some I and original II. III and Br in C6H6 failed to react at room temperature, while at reflux in AcOH some 2,2-dibromo-1,3-indandione, m. 178°, was formed.
CC 10F (Organic Chemistry: Condensed Carbocyclic Compounds)
IT 101278-69-7 111439-41-9

(Derived from data in the 6th Collective Formula Index (1957-1961))
IT 101278-69-7 111439-41-9
(Derived from data in the 6th Collective Formula Index (1957-1961))
RN 101278-69-7 ZCAPLUS
CN Indene-2-carbonitrile, 1-oxo-3-phenyl-, oxime (6CI) (CA INDEX NAME)



RN 111439-41-9 ZCAPLUS
CN Indene-2-carbonitrile, 1-oxo-3-phenyl-, (2,4-dinitrophenyl)hydrazone (6CI) (CA INDEX NAME)



L106 ANSWER 37 OF 40 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1961:48596 ZCAPLUS Full-text
DOCUMENT NUMBER: 55:48596
ORIGINAL REFERENCE NO.: 55:9359g-i,9360a-i
TITLE: Electrophilic properties of ethyl 3-phenylindone-2-carboxylate
AUTHOR(S): Koelsch, C. F.
CORPORATE SOURCE: Univ. of Minnesota, Minneapolis
SOURCE: Journal of Organic Chemistry (1960), 25, 2088-91
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 55:48596

AB In spite of presumed steric hindrance and electronic deactivation, the 2,3-double bond in Et 3-phenylindone-2-carboxylate (I) was quite reactive. The compound added amines or alcs. to give products stable only in basic solution, but it added many other types of active H compds. including HCN, MeNO2, CH2(CO2Et)2 (II), or Me2CO to give relatively stable products. o-Benzoylbenzoylmalonic ester (37 g.) with 100 ml. 5% Na2CO3 refluxed 10 min., cooled, the solution decanted, the product refluxed with 100 ml. H2O, and dried in vacuo gave 26.5 g. I, m. 88-9°. I (0.5 g.), 2 ml. H2O, 0.2 g. NaCN, and a little alc. gave 0.5 g. 2-carbethoxy-3-cyano-3- phenylhydrindone, m. 99-101°, purple with alc. FeCl3, Na salt difficultly soluble in 10% NaOH and not affected by refluxing 1 hr. I (1 g.), 3 ml. Me2CO, and 10 ml. 10% KOH shaken 10 min., excess Me2CO removed (the salt with PhMe became crystalline), and the salt in Et2O shaken with cold HCl gave 1 g. 3-acetonyl-2-carbethoxy-3-phenylhydrindone (III), m. 96-9°, red-purple with alc. FeCl3. III (2.7 g.) with 10 ml. 48% HBr refluxed 10 min. and evaporated gave 2.1 g. crude 3-

acetonyl-3- phenylhydrindone, tan prisms, m. 95-6° (EtOAc-ligroine). I (3 g.), 3 g. cyclohexanone, 6 ml. Me3COH, and 10 ml. 10% NaOH shaken a few min., evaporated to dryness at 100° in vacuo, treated with H2O and Et2O to give the Na salt, the salt dissolved in alc., and made slightly acidic gave 2 g. 2-carbethoxy-3-2-cyclohexanonyl)-3-phenylhydrindone, plates, m. 126-36°, blue with alc. FeCl3. I (3 g.) and 3 g. MeNO2 in 6 ml. Me3COH treated with 5 ml. 10% NaOH, cooled, acidified, and the product recrystd. gave 3 g. 2-carbethoxy-3-nitromethyl-3-phenylhydrindone, m. 105-7°, purple with FeCl3. I (8.4 g.), 5 g. II in 10 Me3COH, and 15 ml. 10% NaOH cooled, treated with Et2O, then ice containing 5 ml. H2SO4, the mixture shaken 0.5 hr., the Et2O layer washed, and evaporated gave 13.2 g. Et 2-carbethoxy-3-phenylhydrindone-3-malonate (IV), m. 89-91° (alc.). IV (13 g.) with 50 ml. 48% HBr refluxed 2 hrs., evaporated, the residue refluxed 1.5 hrs. with 25 ml. fresh HBr and 10 ml. AcOH, the mixture evaporated, the 9.4 g. gum heated at 185° until gas evolution ceased, and crystallized gave 8.2 g. crude acid. The acid taken up in 40 ml. MeOH containing 2 ml. H2SO4 and refluxed 1 hr. gave 7.6 g. Me 3-phenylhydrindone-3-acetate (V), b15 230-5°, m. 88-9° (EtOAc-ligroine). Saponifying V by refluxing 5 min. with 2% KOH gave 3-phenylhydrindone-3-acetic acid, m. 91-2°, recrystd. from CH2Cl2, m. 128-30°. I (0.5 g.) with 0.5 ml. NCCH2CO2Et treated overnight with 1 drop 50% KOH and acidified gave Et 2-carbethoxy-3-phenyl-3-cyanoacetate, m. 121-4° (alc.), purple with FeCl3. I (1 g.) refluxed 1 min. with 10 ml. 10% NaOH and 1 ml. 75% thioglycolic acid and acidified at 0° gave 2-carbethoxy-3-phenylhydrindone-3-thioglycolic acid, m. 105°, purple color with FeCl3, soluble in cold dilute NaHCO3. KOH (0.5 g.) in 5 ml. PhOH was distilled to 2/3 volume, cooled, heated 0.5 min. to 160° with 1 g. I, diluted with Et2O, washed with dilute HCl, evaporated, heated to 160°/10 mm., the residue dissolved in Et2O, and extracted with 5% NaOH; this left 0.05 g. I and removed 1.2 g. phenolic material which crystallized to give Et 3-(p-hydroxyphenyl)-3-phenylhydrindone-2-carboxylate (VI), m. 155-60°, purple-red with FeCl3. VI was easily hydrolyzed and decarboxylated but it was simpler to prepare 3-(p-hydroxyphenyl-3- phenylhydrindone directly. KOH (1 g.) in 10 g. PhOH treated with 2 g. I and the mixture refluxed 5 min. gave the latter product in 1.75-g. yield, m. 136-9° (EtOAc-ligroine), no color with FeCl3. With Me2SO4 in aqueous NaOH, the phenol gave 3-(p-anisyl)-3-phenylhydrindone, prisms, m. 86-8° (MeOH). p-Anisyldiphenylchloromethane (22 g.) in 65 ml. C6H6 mixed with 20 g. ClHgCH2CHO, the mixture stirred 4 hrs. at room temperature, then refluxed 2 hrs., H2O added, the product refluxed 15 min. in 50 ml. Me2CO with 10 g. KMnO4, after an addnl. 45 min. the Me2CO evaporated, and replaced with Et2O and dilute Na2CO3 gave from the aqueous layer 8.6 g. β-(p-anisyl)-β,β-diphenylpropionic acid (VII), plates, m. 156-7° (dilute AcOH). VII with polyphosphoric acid gave only gummy products, but the desired cyclization was achieved as follows. Addition of a drop of C5H5N to 1 g. VII and 5 ml. SOCl2 initiated a reaction; the residue taken up in 5 ml. C6H6, treated 15 min. at room temperature with 1 g. AlCl3, the mixture neutralized, the neutral product kept some time with Et2O-ligroine, and crystallized gave 20 mg. 3-(p-anisyl)-3-phenylhydrindone, m. 87-8° (ligroine). I (1 g.) with 1.5 g. PhNH2 refluxed 5 min. gave 1.1 g. 3-phenylindone-2-carboxanilide, red prisms, m. 178-9°, insol. in hot aqueous NaOH. If refluxing I with PhNH2 was prolonged to 10 min., part of the product was 3-phenyl-indone-2-carboxanilide anil, yellow needles, m. 217-18° (BuOH). The anil with HCl in alc. deposited the anilide. The anilide (1 g.) in 7 ml. alc. treated with 0.5 g. NaCN in a little H2O gave 1 g. 3-cyano-3-phenylhydrindone-2-carboxanilide, tan prisms, m. 157-9° (alc.). purplish red FeCl3 test. I (2.5 g.) in 10 ml. C6H6 treated with 6 ml. 2N PhMgBr and the product treated with dilute HCl gave 2.9 g. tan oil, which could not be crystallized This was treated with 10 ml. 20% MeOH-KOH to give the K salt, which washed, dissolved in H2O, and acidified gave 1,3-diphenyl-1-hydroxyindene-2-carboxylic acid (VIII), m. 163-4° (dilute alc.). VIII (0.5 g.) in 5 ml. AcOH and 1 ml. AcCl treated with 0.5 g. Zn dust under reflux 10

min., H2O added, and the Et2O solution extracted with dilute Na2CO3 gave 50 mg. 1,3-diphenylindene-2-carboxylic acid (IX), yellow needles, m. 195-6° (AcOH). IX, synthesized by refluxing 2 g. 1,3-diphenylindene with 2 ml. (COCl)2 1 hr. m. 173-81°; this in dilute Na2CO3 warmed with 3 ml. 3% H2O2 and repptd. gave IX.

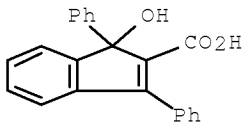
CC 10F (Organic Chemistry: Condensed Carbocyclic Compounds)

IT 976-84-1P, Propionic acid, 3-(p-methoxyphenyl)-3,3-diphenyl- 40413-12-5P, 1-Indanacetic acid, 3-oxo-1-phenyl- 67845-24-3P, Indene-2-carboxylic acid, 1,3-diphenyl- 98117-19-2P, Indene-2-carboxanilide, 1-oxo-3-phenyl- 101723-16-4P, 1-Indanone, 3-acetonyl-3-phenyl- 101723-47-1P, 1-Indanacetic acid, 3-oxo-1-phenyl-, methyl ester 102022-81-1P, 2-Indancarboxylic acid, 1-nitromethyl-3-oxo-1-phenyl-, ethyl ester 102078-31-9P, 1-Indanacetic acid, 2-carboxy-α-mercapto-3-oxo-1-phenyl-, 2-ethyl ester 102242-25-1P, 1-Indanone, 3-(p-hydroxyphenyl)-3-phenyl- 102473-94-9P, 2-Indancarboxylic acid, 1-acetonyl-3-oxo-1-phenyl-, ethyl ester 102663-96-7P, 2-Indancarboxylic acid, 1-(p-hydroxyphenyl)-3-oxo-1-phenyl-, ethyl ester 102705-84-0P, 1-Indanone, 3-(p-methoxyphenyl)-3-phenyl- 102749-23-5P, 2-Indancarboxylic acid, 3-oxo-1-(2-oxocyclohexyl)-1-phenyl-, ethyl ester 102888-54-0P, 1-Indanacetic acid, 2-carboxy-α-cyano-3-oxo-1-phenyl-, diethyl ester 102952-72-7P, 1-Indanmalonic acid, 2-carboxy-3-oxo-1-phenyl-, triethyl ester 103278-17-7P, Indene-2-carboxamidine, 1-oxo-N,N',3-triphenyl- 108478-68-8P, 2-Indancarboxylic acid, 1-cyano-3-oxo-1-phenyl-, ethyl ester 110474-98-1P, Indene-2-carboxylic acid, 1-hydroxy-1,3-diphenyl- 112115-99-8P, 2-Indancarboxanilide, 1-cyano-3-oxo-1-phenyl- 112714-19-9P, Indene-2-carboxylic acid, 1-hydroxy-1,3-diphenyl-, potassium salt
RL: PREP (Preparation)
(preparation of)

IT 110474-98-1P, Indene-2-carboxylic acid, 1-hydroxy-1,3-diphenyl- 112714-19-9P, Indene-2-carboxylic acid, 1-hydroxy-1,3-diphenyl-, potassium salt
RL: PREP (Preparation)
(preparation of)

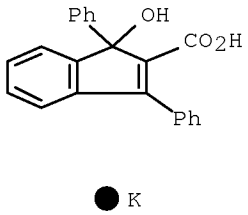
RN 110474-98-1 ZCAPLUS

CN Indene-2-carboxylic acid, 1-hydroxy-1,3-diphenyl- (6CI) (CA INDEX NAME)



RN 112714-19-9 ZCAPLUS

CN Indene-2-carboxylic acid, 1-hydroxy-1,3-diphenyl-, potassium salt (6CI) (CA INDEX NAME)



L106 ANSWER 38 OF 40 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1958:25449 ZCAPLUS Full-text
DOCUMENT NUMBER: 52:25449
ORIGINAL REFERENCE NO.: 52:4586e-i,4587a-h
TITLE: Attempts to prepare new aromatic systems. VI. 1,2,5,6-Dibenzopentalene and derivatives
AUTHOR(S): Baker, Wilson; McOmie, J. F. W.; Parfitt, S. D.; Watkins, D. A. M.
CORPORATE SOURCE: Univ. Briston, UK
SOURCE: Journal of the Chemical Society (1957) 4026-37
CODEN: JCSOA9; ISSN: 0368-1769
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB 2-Benzylideneindan-1,3-dione was added to PhMgBr (from 8.3 g. PhBr) in Et2O, boiled 1 hr., poured into dilute HCl, and on elution from Al2O3 with alc. gave 2-diphenylmethyl-3-phenylinden-1-one (I), m. 154° [differs from Kohler's (C.A. 1, 1849) conclusion that 3,4-dihydro-3-oxo-4- phenyl-1,2,5,6-dibenzopentalene (II) was formed]; 2,4- dinitrophenylhydrazone, m. 249°; oxime, m. 159-62°. 2-(Diphenylmethyl)indan-1,3-dione (III), m. 128-9°, was similarly prepared by using increased amts. of reagents. III and PhMgBr gave I. I with Cr2O3 in HOAc gave Ph2CO and 2-PhCOC6H4CO2H while III gave Ph2CO, Ph2CHCO2H, and phthalic acid. Ph2CHCH(CO2H)2 (2 g.) was heated with 20 g. polyphosphoric acid at 120° 1 hr., poured into H2O, and crystallized from C6H6 to give 3,4,7,8-tetrahydro-3,4-dioxo-1,2,5,6-dibenzopentalene (IV), m. 259°, soluble in hot but not cold aqueous NaOH, gives a CHCl3 soluble green Cu derivative, gives no color with alc. FeCl3, and remains unchanged by Na in hot ethylene glycol; mono-2,4-dinitrophenylhydrazone, m. 297° (decomposition); mono-4-toluenesulfonylhydrazone, m. 116°. 3-Phenylindan-1-one (V) (2,4-dinitrophenylhydrazone, m. 209-10°) and Ph2CHCH2CO2H were prepared from cinnamic acid and AlCl3. V (21 g.) in 50 cc. (EtO)2CO (VI) was added slowly to 150 cc. VI in which 2.3 g. Na was dissolved and heated at 150° to give trans-Et 1-oxo-3-phenylindan-2-carboxylate (VII), m. 103-4°; 2,4-dinitrophenylhydrazone, m. 179°. The ester prepared by Yost (C.A. 45, 2928i) was probably the cis isomer. VII (2 g.) was heated at 160° 3 min. with excess polyphosphoric acid and poured into H2O to give IV. V (10 g.), 9 g. (CO2Et)2, and 40 cc. EtOH was added with stirring to 100 cc. warm EtOH containing 10 g. Na and poured into dilute HCl giving 1-oxo-3-phenyl-2-indanylglyoxylic acid (VIII), m. 213°, and probably 3-phenyl-2-(3-phenyl-1-indenylidene)indan-1-one, m. 185°; Me ester of VIII, m. 148°. Cyclization of VIII with polyphosphoric acid gave IV. IV (1.0 g.), 6 g. Zn-Hg, 20 cc. H2O, 50 cc. concentrated HCl, 1 cc. HOAc, and 5 cc. MePh was refluxed 40 hrs. giving 3,4,7,8-tetrahydro-1,2,5,6-dibenzopentalene (IX), m. 95°. IX (0.2 g. and 0.3 g. chloranil was boiled in 10 cc. C6H6 14 hrs., poured into dilute NaOH, and extracted with Et2O to give 3(or 7)-(2,3,5,6-tetrachloro-4-hydroxyphenoxy)- 1,2,5,6-dibenzopentalene (X), m. 210°. Sublimation of X at 230°/12 mm. gave IX. IV (0.5 g.) and 5 g. PCl5 was heated at 100° 5 min. to give 3,3,4,4,7,8-

hexachloro-3,4,7,8-tetrahydro- 1,2,5,6-dibenzopentalene, m. 207°, and 8(or 7)-chloro-3,4,7,8- tetrahydro-3,4-dioxo-1,2,5,6-dibenzopentalene, m. 172°. IV with LiAlH4 gave 2 stereoisomers of 3,4,7,8-tetrahydro-3,4-dihydroxy-1,2,5,6-dibenzopentalene: isomer A, m. 262° (di-Ac derivative, m. 109-10°; Bz derivative, m. 169°); isomer B, m. 200° (di-Ac derivative, m. 158°). IV (1 g.) in Et2O was boiled with MeMgI and 3,4,7,8-tetrahydro-3-methylene-4-oxo-1,2,5,6-dibenzopentalene (XI), m. 156°; separated XI gives a red solution with concentrated H2SO4. 2-Benzylidene-3-phenylindan-1-one (XIa) (5 g.), 200 cc. C6H6, and 50 g. AlCl3 was refluxed 6 hrs. and poured into H2O giving 3,4,7,8-tetrahydro-3- oxo-4-phenyl-1,2,5,6-dibenzopentalene (XII), m. 132°; 2,4-dinitrophenylhydrazone, m. 271°. To 2.5 g. XII in a warm solution of 1 g. Na in 50 cc. ethylene glycol was added pure N2H4, the mixture refluxed 20 hrs., poured into H2O, and extracted with Et2O to give 3,4,7,8-tetrahydro-3-phenyl-1,2,5,6-dibenzopentalene (XIII), m. 112°. XII (10 g.) and 10 g. PCl5 in 100 cc. C6H6 was boiled 10 hrs., distilled to dryness in vacuo, and crystallized from light petr. giving 3,3-dichloro-3,4,7,8-tetrahydro-4-phenyl-1,2,5,6-dibenzopentalene (XIV), m. 151°, which hydrolyzes in damp air or alc. KOH or reacts with Ag2O in anhydrous C6H6 to give XII. XIV with Zn-HCl gave XIII. When XIV is melted under reduced pressure or boiled in pyridine 45 min., 3,3,4(or 7)-trichloro-3,4,7,8-tetrahydro-4-phenyl-1,2,5,6-dibenzopentalene, m. 214° (decomposition), is obtained. The 4-toluenesulfonylhydrazone of XII, m. 204°, reacts with Na in ethylene glycol to give 3,4,7,8-tetrahydro-3-(2-hydroxyethoxy)-4-phenyl-1,2,5,6-dibenzopentalene, m. 147°, and similarly replacing glycol with cyclohexanol as solvent XII gave 3-cyclohexyloxy-3,4,7,8-tetrahydro-4-phenyl-1,2,5,6- dibenzopentalene, m. 133°. XII with LiAlH4 gave 3,4,7,8-tetrahydro-3-hydroxy-4-phenyl-1,2,5,6-dibenzopentalene (XV), m. 176-8° (Ac derivative, m. 151°), while reduction with Al(OCHMe2)3 gave a 2nd isomer (XVI) of XV, m. 148°; Ac derivative, m. 145°. The Ac derivs. of XV and XVI do not decompose on heating alone or with anhydrous K2CO3. XV (1 g.) and 1 g. anhydrous CuSO4 was boiled 4 hrs. in 30 cc. xylene, then filtered, and the residue washed with Et2O. Evaporation of the filtrate and washings gave 4,7(?)-dihydro-4-phenyl-1,2,5,6- dibenzopentalene (XVII), m. 178-80°, and an unknown compound (XVIII), m. 158-9°. XVII and XVIII were also prepared by heating XV with anhydrous CuSO4 7 hrs., but after 10 hrs. only XVIII was isolated. A similar dehydration of XVI gave XVII after 1.5 hrs. and XVIII after 3 hrs. boiling. When either XV or XVI was heated with P2O5 in C6H6 a substance was formed which melted at about 60°, solidified at about 80°, and then m. 154°, ν 745 and 702 cm.-1 Dry air containing Br and CHCl3 passed through a CHCl3 solution of XII yielded 3,4-dihydro-3-oxo-4-phenyl-1,2,5,6-dibenzopentalene (XIX), m. 266-9° (decomposition). IV and PhMgBr refluxed 1 hr. gave 3,4,7,8-tetrahydro-3-hydroxy-4-oxo-3-phenyl-1,2,5,6-dibenzopentalene (XX), m. 120°. Similarly, IV and excess PhMgBr or PhLi gave XIX and XX. The epoxide of XIa (XXI), m. 164°, was prepared by the reaction of H2O2 with XIa in the presence of NaOH. 1,3-Dihydroxy-2,4- diphenylnaphthalene, n. 163-5°, was prepared by the reaction of XXI with polyphosphoric acid at 160° and 192°, by heating with excess concentrated HCl 3 hrs., or by reaction with BF3. XII and PhMgBr in Et2O boiled 5 hrs. gave 3,4,7,8-tetrahydro-3-hydroxy-3,4-diphenyl-1,2,5,6- dibenzopentalene (XXII), m. 160°. Dehydration of XXII with anhydrous CuSO4 gave 4,7-dihydro-3,4-diphenyl-1,2,5,6-dibenzopentalene (XXIII), m. 202-4°. XXIII in CCl4 with oxides of N prepared from fuming HNO3, H2SO4, and As2O3 gave a crystalline addition compound, C28H20N2O4, m. 242°.

CC 10 (Organic Chemistry)

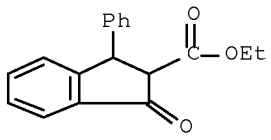
IT 93875-76-4 102754-81-4 103161-86-0 103282-30-0
111474-70-5 111614-43-8 115081-48-6 115101-95-6 115187-93-4
116598-03-9 116665-66-8 124290-46-6 132647-63-3 132647-64-4
(Derived from data in the 6th Collective Formula Index (1957-1961))

IT 606-83-7P, Propionic acid, 3,3-diphenyl- 1821-21-2P, 1,3-Indandione,

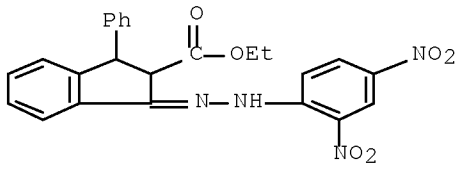
2-diphenylmethyl- 16618-72-7P, 1-Indanone, 3-phenyl- 19546-08-8P, 1,3-Naphthalenediol, 2,4-diphenyl- 21013-44-5P, Indeno[1,2-a]indene, 4b,9,9a,10-tetrahydro- 101445-88-9P, 2-Indanglyoxylic acid, 1-oxo-3-phenyl- 101736-95-2P, 2-Indanglyoxylic acid, 1-oxo-3-phenyl-, methyl ester 103404-05-3P, 1-Indanone, 3-phenyl-2-(3-phenylinden-1-ylidene)-(?) 109339-16-4P, Indeno[1,2-a]inden-9(10H)-one, 4b,9a-dihydro-10-methylene- 110144-58-6P, 1-Indanone, 3-phenyl-, (2,4-dinitrophenyl)hydrazone 112223-51-5P, Indeno[1,2-a]inden-9(10H)-one, 4b,9a-dihydro-10-hydroxy-10-phenyl- 112223-53-7P, Indeno[1,2-a]indene, 4b,9-dihydro-9-phenyl-(?) 112349-28-7P, Spiro[indan-2,2'-oxiran]-1-one, 3,3'-diphenyl- 112991-99-8P, Indeno[1,2-a]indene, 4b,9,9a,10-tetrahydro-9-phenyl- 114863-01-3P, Hydrazine, 1-(4b,9a-dihydro-10-oxoindeno-[1,2-a]inden-9(10H)-ylidene)-2-p-tolylsulfonyl- 115349-53-6P, [Δ1,2'-Biindan]-1'-one, 3,3'-diphenyl- 116604-97-8P, Phenol, 2,3,5,6-tetrachloro-4-(9,10-dihydroindeno[1,2-a]inden-4b(9aH)-yloxy)-(?) 116604-98-9P, Phenol, 2,3,5,6-tetrachloro-4-(4b,9,9a,10-tetrahydroindeno[1,2-a]inden-9-yloxy)-(?) 116665-59-9P, Indeno[1,2-a]inden-9(10H)-one, 10-phenyl- 119014-09-4P, Ethanol, 2-(4b,9,9a,10-tetrahydro-10-phenylindeno[1,2-a]inden-9-yloxy)- 121475-08-9P, Indeno[1,2a]inden-9-ol, 4b,9,9a,10-tetrahydro-9,10-diphenyl- 122447-43-2P, Indeno[1,2-a]indene, 9-(cyclohexyloxy)-4b,9,9a,10-tetrahydro-10-phenyl- 124105-34-6P, Indeno[1,2-a]indene, 4b,9-dihydro-9,10-diphenyl- 124270-58-2P, Hydrazine, 1-(4b,9a-dihydro-10-phenylindeno-[1,2-a]inden-9(10H)-ylidene)-2-p-tolylsulfonyl- 133231-24-0P, Indeno[1,2-a]indene, 4b,9,9,9a,10,10-hexachloro-4b,9,9a,10-tetrahydro- 440114-83-0P, 2-Indancarboxylic acid, 1-oxo-3-phenyl-, trans-, ethyl ester 856641-92-4P, 2-Indancarboxylic acid, 1-oxo-3-phenyl-, (2,4-dinitrophenyl)hydrazone
RL: PREP (Preparation)
(preparation of)

IT 93875-76-4 102754-81-4
(Derived from data in the 6th Collective Formula Index (1957-1961))

RN 93875-76-4 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 2,3-dihydro-1-oxo-3-phenyl-, ethyl ester (CA INDEX NAME)

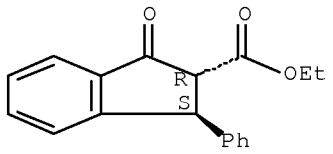


RN 102754-81-4 ZCAPLUS
CN 2-Indancarboxylic acid, 1-oxo-3-phenyl-, ethyl ester, (2,4-dinitrophenyl)hydrazone (6CI) (CA INDEX NAME)

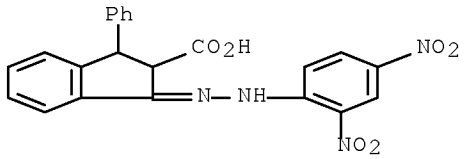


IT 440114-83-0P, 2-Indancarboxylic acid, 1-oxo-3-phenyl-, trans-, ethyl ester 856641-92-4P, 2-Indancarboxylic acid, 1-oxo-3-phenyl-, (2,4-dinitrophenyl)hydrazone
RL: PREP (Preparation)
(preparation of)
RN 440114-83-0 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 2,3-dihydro-1-oxo-3-phenyl-, ethyl ester, (2R,3S)-rel- (CA INDEX NAME)

Relative stereochemistry.



RN 856641-92-4 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-[2-(2,4-dinitrophenyl)hydrazinylidene]-2,3-dihydro-3-phenyl- (CA INDEX NAME)



L106 ANSWER 39 OF 40 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1958:25448 ZCAPLUS Full-text
DOCUMENT NUMBER: 52:25448
ORIGINAL REFERENCE NO.: 52:4586a-e
TITLE: Attempts to prepare new aromatic systems. V. Benzopentalene (cyclopent[a]indene)
AUTHOR(S): Baker, Wilson; McOmie, J. F. W.; Ulbricht, T. L. V.
CORPORATE SOURCE: Univ. Briston, UK
SOURCE: Journal of the Chemical Society (1957) 4022-5
CODEN: JCSOA9; ISSN: 0368-1769
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB cf. C.A. 46, 8075h. To a CS2 solution of 3-oxo-2-phenylcyclopentane-1-carboxylic acid, fluorosulfonic acid was added, yielding 3,4,5,6,7,8-hexahydro-3,6-dioxobenzopentalene (I), m. 86-8°; bis-2,4-dinitrophenylhydrazone, m. 277° (decomposition); piperonylidene derivative, m. 181-2°. I (0.25 g.), 0.10 g. Br, and 10 ml. CHCl3 was refluxed 3 hrs. and the solvent removed to give 5,5,7,8(?)-tetrabromo- 3,4,5,6,7,8-hexahydro-3,6-dioxobenzopentalene, m. 147-8°. 4,5-Dihydro-3,6-diphenylbenzopentalene (II), m. 180°, was prepared in 74% yield from I and excess PhMgBr. II and Br in CHCl3 gave 4(or 5)-bromo-4,5-dihydro-3,6-diphenylbenzopentalene, m. 208-10°

(decomposition). II (0.4 g.) was heated with 0.24 g. N-bromosuccinimide (III) and 0.6 g. BaCO3 in CCl4 1 hr., then cooled, filtered, and the filtrate heated with 10 ml. PhNMe2 1.5 hrs. and 5 ml. pyridine 0.5 hr., dissolved in H2O and washed with 5N HCl and H2O to give bi[4,5-dihydro-3,6- diphenylbenzopentalen-4(or 5)-yl], m. 277° (decomposition). I and PCl5 gave 3,6-dichloro-4,5-dihydrobenzopentalene (IV), m. 117-17.5°, 6,6,7(or 8)-trichloro-3,4,5,6,7,8-hexahydro-3-oxobenzopentalene, m. 108-9°, and a yellow compound, m. 241-2° (decomposition). IV (0.3 g.), 0.25 g. III, and 0.01 g. Bz2O2 in 20 ml. CCl4 refluxed 4 hrs., filtered, washed with 2N NaOH and H2O, and the solvent removed gave an oil which gave on crystallization from MeOH 3,6-dichloro-4,5-dihydro-4(or 5)-methoxybenzopentalene, m. 96°. III, IV, and Bz2O2 in CCl4 was refluxed 1 hr., the solvent removed from the filtrate, the residual oil boiled a few min. with KOAc in HOAc, evaporated, and poured into H2O. Extraction with Et2O gave 4(or 5)-acetoxy-3,6-dichloro-4,5-dihydrobenzopentalene (V), m. 117-8°. When V was heated at about 500°/4 × 10-3 mm., very little decomposition resulted, but V was decomposed by heating just above its m.p. with anhydrous K2CO3.

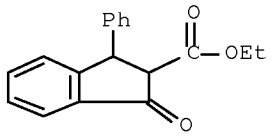
CC 10 (Organic Chemistry)

IT 2717-47-7 6938-36-9 93875-76-4 94254-93-0 101594-37-0
102754-81-4 103161-86-0 103282-30-0 107414-32-4
109188-49-0 111474-70-5 111614-43-8 114003-55-3 115081-48-6
115101-95-6 115187-93-4 116598-03-9 116665-66-8 124290-46-6
132647-63-3 132647-64-4
(Derived from data in the 6th Collective Formula Index (1957-1961))

IT 93875-76-4 102754-81-4
(Derived from data in the 6th Collective Formula Index (1957-1961))

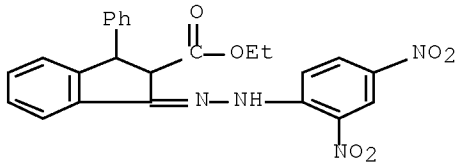
RN 93875-76-4 ZCAPLUS

CN 1H-Indene-2-carboxylic acid, 2,3-dihydro-1-oxo-3-phenyl-, ethyl ester (CA INDEX NAME)



RN 102754-81-4 ZCAPLUS

CN 2-Indancarboxylic acid, 1-oxo-3-phenyl-, ethyl ester, (2,4-dinitrophenyl)hydrazone (6CI) (CA INDEX NAME)



L106 ANSWER 40 OF 40 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1955:39399 ZCAPLUS Full-text
DOCUMENT NUMBER: 49:39399

ORIGINAL REFERENCE NO.: 49:7539c-i
TITLE: Dimeric cinnamic acids and alcohols
AUTHOR(S): Freudenberg, Karl; Schuhmacher, Gunter
CORPORATE SOURCE: Univ. Heidelberg, Germany
SOURCE: Chemische Berichte (1954), 87, 1882-7
CODEN: CHBEAM; ISSN: 0009-2940
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
GI For diagram(s), see printed CA Issue.

AB 3,4 (MeO)2C6H3CH:CHCO2Et with LiAlH4 at below 0° gave 87% 3,4-(MeO)2C6H3CH:CHCH2OH (I), needles, m. 78° (from H2O-MeOH); it polymerized in concentrated HCl. A melt of 6 g. 3,4-(MeO)2C6H3CH:CHCO2Me and 2 drops 20% aqueous HClO4 heated 14 h. on a water bath gave 42% dimer (II, R = CO2Me, R' = Me), needles, m. 142-2.5° (from MeOH); from the mother liquors was isolated 25% of a dimorphic or stereoisomeric form, rods, m. 127-8°. Similarly, Et ferulate was dimerized to 20% II (R = CO2Et, R' = H), rods, m. 156.5-7.5° diacetate, plates, m. 98-8.5° (from BuOH). II (R = CO2Me, R' = Me) (5 g.) and 1.5 g. LiAlH4 in THF gave 73% dimer (IIa) of I (II, R = CH2OH, R' = Me), m. 150-1° after recrystn. from C6H6 and drying at 120° in vacuo; dimethanesulfonate, needles, m. 155-6° (from Me2CO-H2O). The di-p-tosylate (2 g.) of IIa and 3.5 g. NaI in 30 cc. absolute Me2CO refluxed 24 h. gave 72% II (R = CH2I, R' = Me), prisms, m. 151.5-2° (from MeOH); this (1 g.) in 90 cc. MeOH and 10 cc. H2O with 3 g. 20% Pd-BaSO4 catalyst under H gave 76% diisoeugenol di-Me ether (II, R = R' = Me), m. 105.5-6.5° (from MeOH-H2O). II (R = CO2Me, R' = Me) (3 g.) in 100 cc. HOAc oxidized with 3 g. CrO3 in 25 cc. HOAc and 5 cc. H2O 14 h. at 20° and the neutral product crystallized from MeOH gave 29% diketone [2,3,4-MeO2CCH2CO(MeO)2C6H2CH[C6H3(OMe)2-3,4]COCO2Me or 2,4,5-[3,4-(MeO)2C6H3CO](MeO)2C6H2CH(CH2CO2Me)COCO2Me}, m. 182.5-3°; UV maximum (neutral medium) at 236, 282, and 318 mμ; (acid medium, H2SO4-HOAc) at 265, 332, 365, 465, and 600 mμ, indicative of the formation of a benzopyrylium compound From the MeOH mother liquors was isolated an amorphous ketone (III) which gave a crystalline 2,4-dinitrophenylhydrazone, red, m. 249-50°. From the acid fraction of the oxidation reaction mixture was isolated o-veratroylveratric acid, m. 221-2°. These oxidation products are analogous to those obtained by A. Muller (C.A. 39, 2745.1) by the oxidation of II (R, R' = Me).

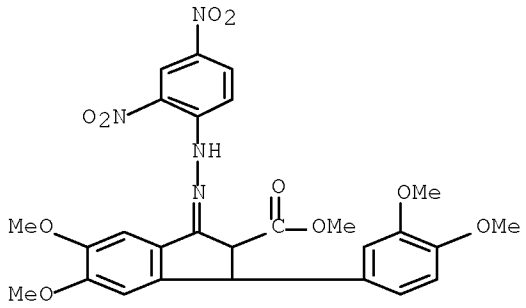
CC 10 (Organic Chemistry)

IT 4483-47-0P, Diisoeugenol, dimethyl ether 4483-47-0P, Indan, 1-(3,4-dimethoxyphenyl)-3-ethyl-5,6-dimethoxy-2-methyl- 7249-36-7P, Veratric acid, 6-veratroyl- 18523-76-7P, 2-Propen-1-ol, 3-(3,4-dimethoxyphenyl)- 412315-66-3P, 1-Indanethanol, 3-(3,4-dimethoxyphenyl)-2-(hydroxymethyl)-5,6-dimethoxy- 412315-67-4P, 1-Indanethanol, 3-(3,4-dimethoxyphenyl)-2-(hydroxymethyl)-5,6-dimethoxy-, dimethanesulfonate 412315-67-4P, Methanesulfonic acid, diester with 3-(3,4-dimethoxyphenyl)-2-(hydroxymethyl)-5,6-dimethoxy-1-indanethanol 412315-94-7P, 1-Indanacetic acid, 2-carboxy-3-(3,4-dimethoxyphenyl)-5,6-dimethoxy-, dimethyl ester 858224-88-1P, Indan, 1-(3,4-dimethoxyphenyl)-3-(2-iodoethyl)-2-(iodomethyl)-5,6-dimethoxy- 858496-04-5P, o-Benzenedipropionic acid, β-(3,4-dimethoxyphenyl)-4,5-dimethoxy-α,β'-dioxo-, dimethyl ester 858496-04-5P, Pyruvic acid, (2-carboxyacetyl-4,5-dimethoxyphenyl)(3,4-dimethoxyphenyl)-, dimethyl ester 859307-10-1P, Glutaric acid, 3-(3,4-dimethoxyphenyl)-2-oxo-3-veratroyl-, dimethyl ester 860355-88-0P, 2-Indancarboxylic acid, 1-(3,4-dimethoxyphenyl)-5,6-dimethoxy-3-oxo-, methyl ester, 2,4-dinitrophenylhydrazone 860355-89-1P, 2-Indancarboxylic acid, 1-(3,4-dimethoxyphenyl)-5,6-dimethoxy-3-oxo-, methyl ester
RL: PREP (Preparation)
(preparation of)

IT 860355-88-0P, 2-Indancarboxylic acid, 1-(3,4-dimethoxyphenyl)-5,6-dimethoxy-3-oxo-, methyl ester, 2,4-dinitrophenylhydrazone
860355-89-1P, 2-Indancarboxylic acid, 1-(3,4-dimethoxyphenyl)-5,6-dimethoxy-3-oxo-, methyl ester
RL: PREP (Preparation)
(preparation of)

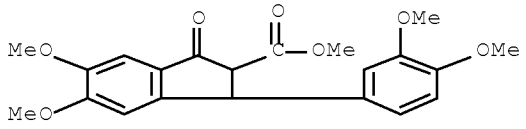
RN 860355-88-0 ZCAPLUS

CN 1H-Indene-2-carboxylic acid, 1-(3,4-dimethoxyphenyl)-3-[2-(2,4-dinitrophenyl)hydrazinylidene]-2,3-dihydro-5,6-dimethoxy-, methyl ester (CA INDEX NAME)



RN 860355-89-1 ZCAPLUS

CN 1H-Indene-2-carboxylic acid, 1-(3,4-dimethoxyphenyl)-2,3-dihydro-5,6-dimethoxy-3-oxo-, methyl ester (CA INDEX NAME)



=> s L102 and L28,L42,L81
L107 3 L102 AND (L28 OR L42 OR L81)

=> d ibib abs hitind hitstr L107 1-3

L107 ANSWER 1 OF 3 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2008:411947 ZCAPLUS Full-text
DOCUMENT NUMBER: 148:427397
TITLE: Novel polybenzofulvene derivatives, synthesis and uses thereof
INVENTOR(S): Cappelli, Andrea; Galeazzi, Simone; Anzini, Maurizio; Vomero, Salvatore
PATENT ASSIGNEE(S): Universita Degli Studi di Siena, Italy
SOURCE: PCT Int. Appl., 47pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2008037604	A1	20080403	WO 2007-EP59698	20070914

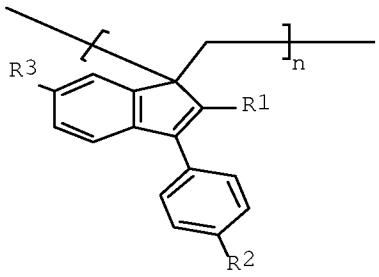
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BH, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DO, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LY, MA, MD, ME, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW

RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, MT, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

PRIORITY APPLN. INFO.: US 2006-846915P P 20060925

OTHER SOURCE(S): CASREACT 148:427397

GI



I

AB The present invention relates to polymers of formula poly-3 (I), their synthesis, intermediates and uses thereof; wherein R1 is H, CH3, CN, a halogen, COOR; R = H, a C1-5 alkyl group, or -(CH2-CH2O)m-CH3, a substituted ethynyl group, or an alkyl group; m is 3-15; R2 and R3 represent a hydrogen atom, a halogen atom, an alkyl group or a hydroxyl group; n is 1-10,000. The invention also related to a pharmaceutical formulation comprising the polymer as drug controlled release pharmaceutical formulation.

CC 35-4 (Chemistry of Synthetic High Polymers)
Section cross-reference(s): 63

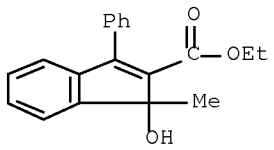
IT 6048-68-6P, Nonaethylene glycolmono methyl ether 13093-22-6P, 2-Chloro-3-phenyl-1H-1-indenone 13304-52-4P, 2-Methyl-3-phenyl-1H-1-indenone 19772-61-3P, 2-Bromo-3-phenyl-1H-1-indenone 35491-56-6P, 1-Oxo-3-phenyl-1H-2-indenecarbonitrile 41916-15-8P, 3-Phenyl-1H-1-indenone 72593-77-2P, 1-Bromo-2-(2-(2-methoxyethoxy)ethoxy)ethane 94224-67-6P, Ethyl 1-Oxo-3-phenyl-1H-2-indenecarboxylate 150192-43-1P, 3-Phenyl-2-(trimethylsilyl)-1H-1-indenone 168007-89-4P, 1-Methylene-3-phenyl-1H-indene 222041-22-7P, 1,2-Dimethyl-3-phenyl-1H-1-indenol 696661-22-0P, 3-(4-Methylphenyl)-1-oxo-1H-2-indenecarbonitrile 724776-29-8P, Ethyl 1-Hydroxy-1-methyl-3-phenyl-1H-indene-2-carboxylate 850209-49-3P, Ethyl 6-methoxy-1-oxo-3-phenyl-1H-indene-2-

carboxylate 867214-96-8P, Ethyl 1-Hydroxy-1-methyl-6-methoxy-3-phenyl-1H-indene-2-carboxylate 937079-93-1P, Ethyl (Z)-2-cyano-3-(4-methylphenyl)-3-phenyl-2-propenoate 937079-95-3P, (E)-2-Cyano-3-(4-methylphenyl)-3-phenyl-2-propenoic acid 937079-96-4P, (Z)-2-Cyano-3-(4-methylphenyl)-3-phenyl-2-propenoic acid 937079-97-5P, 6-Methyl-1-oxo-3-phenyl-1H-2-indenecarbonitrile 937079-98-6P, 3-Phenyl-2-[2-(2-pyridyl)-1-ethynyl]-1H-1-indenone 937080-00-7P, 1-Methyl-3-phenyl-1H-1-indenol 937080-01-8P, 1-Methyl-3-phenyl-2-(trimethylsilyl)-1H-1-indenol 937080-02-9P, 2-Chloro-1-methyl-3-phenyl-1H-1-indenol 937080-04-1P, 2-Bromo-1-methyl-3-phenyl-1H-1-indenol 937080-09-6P, 1-Hydroxy-1-methyl-3-(4-methylphenyl)-1H-indene-2-carbonitrile 937080-10-9P, 1,6-Dimethyl-1-hydroxy-3-phenyl-1H-indene-2-carbonitrile 937080-11-0P, 1-Methyl-3-phenyl-2-2-(2-pyridyl)-1-ethynyl]-1H-1-indenol 937080-18-7P, 2-Fluoro-1-methyl-3-phenyl-1H-1-indenol 937080-19-8P, 2-Fluoro-1-methylene-3-phenyl-1H-indene 937080-20-1P, 2-Chloro-1-methylene-3-phenyl-1H-indene 937080-21-2P, 2-Bromo-1-methylene-3-phenyl-1H-indene 937080-22-3P, 2-Methyl-1-methylene-3-phenyl-1H-indene 937080-23-4P, 1-Methylene-3-phenyl-1H-indene-2-carbonitrile 937080-24-5P, 1-Methylene-3-(4-methylphenyl)-1H-indene-2-carbonitrile 937080-25-6P, 6-Methyl-1-methylene-3-phenyl-1H-indene-2-carbonitrile 937080-26-7P, Ethyl 1-methylene-3-phenyl-1H-indene-2-carboxylate 937080-32-5P, 1-Methylene-3-phenyl-2-[2-(2-pyridyl)-1-ethynyl]-1H-indene 1016567-36-4P, 2-[2-(2-Methoxyethoxy)ethoxyl]ethyl 3-(4-Methylphenyl)-1-oxo-1H-indene-2-carboxylate 1016567-41-1P 1016567-46-6P, [2-[2-(2-Methoxyethoxy)ethoxyl]ethyl 1-Hydroxy-1-methyl-3-(4-methylphenyl)-1H-indene-2-carboxylate 1016567-48-8P, 2,5,8,11,14,17,20,23,26-Nonaoxaoctacosan-28-yl 1-hydroxy-1-methyl-3-(4-methylphenyl)-1H-indene-2-carboxylate 1016567-53-5P, [2-[2-(2-Methoxyethoxy)ethoxy]ethyl 1-Methylene-3-(4-methylphenyl)-1H-indene-2-carboxylate 1016567-55-7P, 2,5,8,11,14,17,20,23,26-Nonaoxaoctacosan-28-yl 1-methylene-3-(4-methylphenyl)-1H-indene-2-carboxylate 1016567-57-9P, Ethyl 1-Methylene-6-methoxy-3-phenyl-1H-indene-2-carboxylate
RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(production of polybenzofulvene derivs. for pharmaceutical formulation)

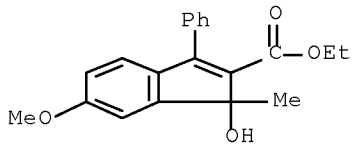
IT 64-17-5, Ethanol, reactions 85-52-9, 2-Benzoylbenzoic acid 105-56-6, Ethyl cyanoacetate 112-35-6, Triethylene glycol monomethyl ether 134-84-9, 4-Methylbenzophenone 594-27-4 1945-84-2, 2-Ethynylpyridine 2170-06-1, 1-Phenyl-2-(trimethylsilyl)acetylene 2615-15-8, Hexaethylene glycol 6630-33-7, 2-Bromobenzaldehyde 696661-26-4, 3-(4-Methylphenyl)-1-oxo-1H-indene-2-carboxylic acid 937080-07-4 , 1-Hydroxy-1-methyl-3-phenyl-1H-indene-2-carbonitrile
RL: RCT (Reactant); RACT (Reactant or reagent)
(production of polybenzofulvene derivs. for pharmaceutical formulation)

IT 724776-29-8P, Ethyl 1-Hydroxy-1-methyl-3-phenyl-1H-indene-2-carboxylate 867214-96-8P, Ethyl 1-Hydroxy-1-methyl-6-methoxy-3-phenyl-1H-indene-2-carboxylate 937080-09-6P, 1-Hydroxy-1-methyl-3-(4-methylphenyl)-1H-indene-2-carbonitrile 1016567-46-6P, [2-[2-(2-Methoxyethoxy)ethoxyl]ethyl 1-Hydroxy-1-methyl-3-(4-methylphenyl)-1H-indene-2-carboxylate 1016567-48-8P, 2,5,8,11,14,17,20,23,26-Nonaoxaoctacosan-28-yl 1-hydroxy-1-methyl-3-(4-methylphenyl)-1H-indene-2-carboxylate
RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(production of polybenzofulvene derivs. for pharmaceutical formulation)

RN 724776-29-8 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-hydroxy-1-methyl-3-phenyl-, ethyl ester (CA INDEX NAME)



RN 867214-96-8 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-hydroxy-6-methoxy-1-methyl-3-phenyl-, ethyl ester (CA INDEX NAME)



RN 937080-09-6 ZCAPLUS
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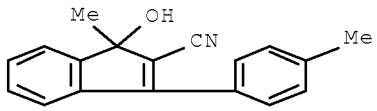
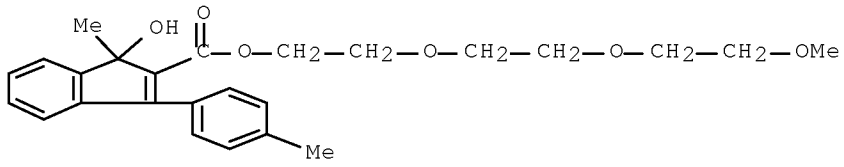
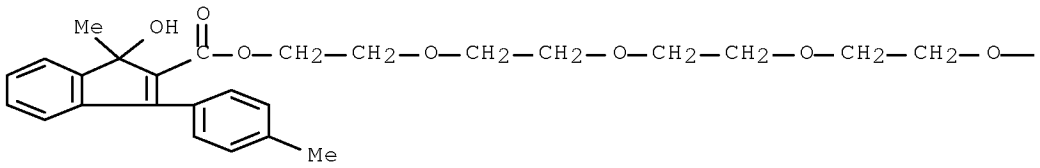


RN 1016567-46-6 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-hydroxy-1-methyl-3-(4-methylphenyl)-, 2-[2-(2-methoxyethoxy)ethoxy]ethyl ester (CA INDEX NAME)

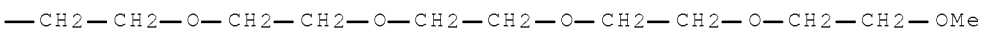


RN 1016567-48-8 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-hydroxy-1-methyl-3-(4-methylphenyl)-, 3,6,9,12,15,18,21,24,27-nonaoxaoctacos-1-yl ester (CA INDEX NAME)

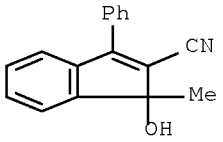
PAGE 1-A



PAGE 1-B



IT 937080-07-4, 1-Hydroxy-1-methyl-3-phenyl-1H-indene-2-carbonitrile
RL: RCT (Reactant); RACT (Reactant or reagent)
(production of polybenzofulvene derivs. for pharmaceutical formulation)
RN 937080-07-4 ZCAPLUS
CN 1H-Indene-2-carbonitrile, 1-hydroxy-1-methyl-3-phenyl- (CA INDEX NAME)



REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L107 ANSWER 2 OF 3 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2007:1388077 ZCAPLUS Full-text
TITLE: Pharmacophore modeling and parallel screening for PPAR ligands
AUTHOR(S): Markt, Patrick; Schuster, Daniela; Kirchmair, Johannes; Laggner, Christian; Langer, Thierry
CORPORATE SOURCE: Department of Pharmaceutical Chemistry, Institute of Pharmacy and Center for Molecular Biosciences Innsbruck (CMBI), University of Innsbruck, Innsbruck, 6020, Austria
SOURCE: Journal of Computer-Aided Molecular Design (2007), 21(10-11), 575-590
CODEN: JCADEQ; ISSN: 0920-654X
PUBLISHER: Springer
DOCUMENT TYPE: Journal
LANGUAGE: English
AB We describe the generation and validation of pharmacophore models for PPARs, as well as a large scale validation of the parallel screening approach by screening PPAR ligands against a large database of structure-based models. A large test set of 357 PPAR ligands was screened against 48 PPAR models to determine the best models for agonists of PPAR-α, PPAR-δ, and PPAR-γ.

Afterwards, a parallel screen was performed using the 357 PPAR ligands and 47 structure-based models for PPARs, which were integrated into a 1537 models comprising inhouse pharmacophore database, to assess the enrichment of PPAR ligands within the PPAR hypotheses. For these purposes, we categorized the 1537 database models into 181 protein targets and developed a score that ranks the retrieved targets for each ligand. Thus, we tried to find out if the concept of parallel screening is able to predict the correct pharmacol. target for a set of compds. The PPAR target was ranked first more often than any other target. This confirms the ability of parallel screening to forecast the pharmacol. active target for a set of compds.

CC 1-3 (Pharmacology)
Section cross-reference(s): 6

ST peroxisome proliferator activated receptor ligand structure virtual screening pharmacophore

IT Structure-activity relationship
(antidiabetic; pharmacophore modeling and parallel screening for PPAR ligands)

IT Structure-activity relationship
(hypolipemic; pharmacophore modeling and parallel screening for PPAR ligands)

IT Antidiabetic agents
Antiobesity agents
Diabetes mellitus
Drug targets
Hyperlipidemia
Hypolipemic agents
Molecular association
Molecular modeling
Obesity
Pharmacophores
(pharmacophore modeling and parallel screening for PPAR ligands)

IT Peroxisome proliferator-activated receptors
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(pharmacophore modeling and parallel screening for PPAR ligands)

IT Structure-activity relationship
(receptor-binding; pharmacophore modeling and parallel screening for PPAR ligands)

IT Drug screening
(virtual; pharmacophore modeling and parallel screening for PPAR ligands)

IT Peroxisome proliferator-activated receptors
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(α; pharmacophore modeling and parallel screening for PPAR ligands)

IT Peroxisome proliferator-activated receptors
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(γ; pharmacophore modeling and parallel screening for PPAR ligands)

IT Peroxisome proliferator-activated receptors
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(δ; pharmacophore modeling and parallel screening for PPAR ligands)

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50892-23-4 79558-09-1 96207-25-9 122320-47-2 122320-74-5
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RL: PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(pharmacophore modeling and parallel screening for PPAR ligands)

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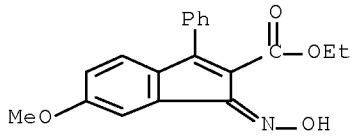
RL: PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(pharmacophore modeling and parallel screening for PPAR ligands)

IT 867215-17-6
RL: PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(pharmacophore modeling and parallel screening for PPAR ligands)

RN 867215-17-6 ZCAPLUS

CN 1H-Indene-2-carboxylic acid, 1-(hydroxyimino)-6-methoxy-3-phenyl-, ethyl ester (CA INDEX NAME)



REFERENCE COUNT: 46 THERE ARE 46 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L107 ANSWER 3 OF 3 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2005:1154511 ZCAPLUS Full-text
DOCUMENT NUMBER: 143:405636
TITLE: Preparation of indenes as selective modulators of peroxisome proliferator activated receptors
PATENT ASSIGNEE(S): Korea Research Institute of Chemical Technology, S. Korea; Jeil Pharm. Co., Ltd.; Korea Research Institute of Bioscience and Biotechnology; Cj Corp.; Cheon, Hyae Gyeong; Yoo, Sung-Eun; Kim, Sung Soo; Yang, Sung-Don; Kim, Kwang-Rok; et al.
SOURCE: PCT Int. Appl., 63 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005100297	A1	20051027	WO 2005-KR1051	20050412

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW

RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

KR 2005100052	A	20051018	KR 2004-25218	20040413
AU 2005233038	A1	20051027	AU 2005-233038	20050412
AU 2005233038	B2	20080313		
CA 2562951	A1	20051027	CA 2005-2562951	20050412
EP 1756036	A1	20070228	EP 2005-733516	20050412
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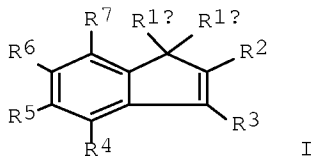
CN 1942427	A	20070404	CN 2005-80011149	20050412
BR 2005009869	A	20071016	BR 2005-9869	20050412
JP 2007532633	T	20071115	JP 2007-508272	20050412
MX 2006PA11514	A	20070802	MX 2006-PA11514	20061005
US 20070225288	A1	20070927	US 2006-599913	20061023
IN 2006DN06489	A	20070831	IN 2006-DN6489	20061102

PRIORITY APPLN. INFO.: KR 2004-25218 A 20040413
WO 2005-KR1051 W 20050412

OTHER SOURCE(S): CASREACT 143:405636; MARPAT 143:405636

GI



I

AB The inventive indenes (shown as I; variables defined below; e.g. 1-hydroxy-6-methoxy-1,3-diphenyl-1H-indene-2-carboxylic acid Et ester (II)) are capable of selectively modulating the activities of peroxisome proliferator activated receptors (PPARs), causing no adverse side effects, and thus, they are useful for the treatment and prevention of disorders modulated by PPARs, i.e., metabolic syndromes such as diabetes, obesity, arteriosclerosis, hyperlipidemia, hyperinsulinism and hypertension, inflammatory diseases such as osteoporosis, liver cirrhosis and asthma, and cancer. Methods of preparation are claimed and .apprx.30 example prepns. are included. For example, II was prepared in 2 steps (72 and 76 % yields) by oxidation of 6-methoxy-3-phenyl-1H-indene-2-carboxylic acid Et ester (preparation given) with SeO2 to give 6-methoxy-1-oxo-3-phenyl-1H-indene-2-carboxylic acid Et ester, which was reacted with phenylmagnesium chloride. EC50 values for activation of PPARγ are tabulated for 15 examples of I; they exhibited superior activation over rosiglitazone. 1-Hydroxy-6-[2- (morpholin-4-yl)ethoxy]-1,3-diphenyl-1H-indene-2-carboxylic acid Et ester hydrochloride was tested for effectiveness in lowering blood glucose level in ob/ob mice; it has an excellent effect in lowering both blood glucose and insulin levels, when it is administered by either orally or i.p. with no side effects such as weight gain, hepatotoxicity or cardiotoxicity. For I: R1a is OH or H; R1b is C1-6 alkyl, C3-6 cycloalkyl, benzyl or Ph ((un)substituted with ≥1 halogen, CN, NH2, NO2 and ORa), when R1a is OH; when R1a is H, R1b is ORa, NRbRc, NHCORa, morpholino, thiomorpholino, or 4-Rapiperazino; R2 is CN, CO2Ra or CONReRf; R3 is Ph (un)substituted with ≥1 halogen, CN, NH2, NO2, ORa and C1-6 alkyl; and R4, R5, R6 and R7 = H, O(CH2)mRg or CH2Rh; in which Ra is H, C1-6 alkyl or C3-

6 cycloalkyl, the C1-6 alkyl and C3-6 cycloalkyl being (un)substituted with ≥1 halogens; Rb, Rc, Re and Rf = H, C1-6 alkyl, C3-6 cycloalkyl or benzyl; Rg is H, Ra-substituted pyridinyl, morpholino, thiomorpholino, 4-Rapiperazino, or Ph, the Ph being (un)substituted with ≥1 halogen, CN, NH2 and NO2; Rh is morpholino, thiomorpholino, or 4-Rapiperazino; and m = 1-3.

IC ICM C07C069-753

CC 24-7 (Alicyclic Compounds)
Section cross-reference(s): 1, 2, 63

ST indene prepn selective modulator peroxisome proliferator activated receptor

IT Heart
Liver
(lack of toxicity of potential drug; preparation of indenes as selective modulators of peroxisome proliferator activated receptors)

IT Cardiotoxicity
Drug toxicity
Hepatotoxicity
(lack of; preparation of indenes as selective modulators of peroxisome proliferator activated receptors)

IT Peroxisome proliferator-activated receptors
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(modulators; preparation of indenes as selective modulators of peroxisome proliferator activated receptors)

IT Antiarteriosclerotics
Antiasthmatics
Antidiabetic agents
Antihypertensives
Antiobesity agents
Antitumor agents
Arteriosclerosis
Asthma
Cirrhosis
Diabetes mellitus
Drug delivery systems
Human
Hypertension
Hypolipemic agents
Neoplasm
Obesity
Osteoporosis
Hyperlipidemia
RL: BIOL (Biological study)
(preparation of indenes as selective modulators of peroxisome proliferator activated receptors)

IT Peroxisome proliferator-activated receptors
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(γ, modulators; preparation of indenes as selective modulators of peroxisome proliferator activated receptors)

IT 867214-93-5P, 1-Hydroxy-6-methoxy-1,3-diphenyl-1H-indene-2-carboxylic acid ethyl ester 867214-96-8P, 1-Hydroxy-6-methoxy-1-methyl-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867214-97-9P, 1-Benzyl-1-hydroxy-6-methoxy-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867214-98-0P, 1-Cyclohexyl-1-hydroxy-6-methoxy-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867214-99-1P, 1-Hydroxy-1,3-diphenyl-6-(3-phenylpropoxy)-1H-indene-2-carboxylic acid ethyl ester 867215-16-5P, 1-Amino-6-methoxy-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867215-18-7P, 1-Amino-3-phenyl-6-(3-phenylpropoxy)-1H-indene-2-carboxylic acid ethyl ester 867215-19-8P, 1-Amino-6-[2-(morpholin-4-yl)ethoxy]-3-

phenyl-1H-indene-2-carboxylic acid cyclohexylamide
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(drug candidate; preparation of indenes as selective modulators of peroxisome proliferator activated receptors)

IT 867187-97-1P, 1-Hydroxy-6-[2-(morpholin-4-yl)ethoxy]-1,3-diphenyl-1H-indene-2-carboxylic acid ethyl ester hydrochloride 867214-94-6P, 1-Hydroxy-6-methoxy-1-(3-methoxyphenyl)-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867214-95-7P, 1-Hydroxy-1-isopropyl-6-methoxy-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867215-00-7P, 1-Hydroxy-6-[2-(morpholin-4-yl)ethoxy]-1,3-diphenyl-1H-indene-2-carboxylic acid ethyl ester 867215-01-8P, 1-Hydroxy-6-[(morpholin-4-yl)methyl]-1,3-diphenyl-1H-indene-2-carboxylic acid ethyl ester 867215-02-9P, 1-Hydroxy-1,3-diphenyl-6-[2-(pyridin-2-yl)ethoxy]-1H-indene-2-carboxylic acid ethyl ester 867215-04-1P, 1-Hydroxy-1,3-diphenyl-6-(3-phenylpropoxy)-1H-indene-2-carbonitrile 867215-07-4P, 1-Hydroxy-1,3-diphenyl-6-(3-phenylpropoxy)-1H-indene-2-carboxylic acid methyl ester 867215-08-5P, 1-Hydroxy-6-methoxy-1,3-diphenyl-1H-indene-2-carboxylic acid 867215-09-6P, 1-Hydroxy-6-methoxy-1-methyl-3-phenyl-1H-indene-2-carboxylic acid 867215-10-9P, 1-Benzyl-1-hydroxy-6-methoxy-3-phenyl-1H-indene-2-carboxylic acid 867215-11-0P, 1-Hydroxy-1,3-diphenyl-6-(3-phenylpropoxy)-1H-indene-2-carboxylic acid 867215-12-1P, 1-Cyclohexyl-1-hydroxy-6-methoxy-3-phenyl-1H-indene-2-carboxylic acid 867215-13-2P, 1,6-Dimethoxy-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867215-15-4P, 1-Ethoxy-6-methoxy-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867215-25-6P, 1-Amino-3-phenyl-6-(3-phenylpropoxy)-1H-indene-2-carbonitrile 867215-27-8P, 1-Acetylamino-6-methoxy-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867215-28-9P, 6-Methoxy-3-phenyl-1-propionylamino-1H-indene-2-carboxylic acid ethyl ester 867215-29-0P, 1-Acetylamino-3-phenyl-6-(3-phenylpropoxy)-1H-indene-2-carboxylic acid ethyl ester 867215-30-3P, 1-Acetylamino-6-[2-(morpholin-4-yl)ethoxy]-3-phenyl-1H-indene-2-carboxylic acid cyclohexylamide 867215-31-4P, 1-Diethylamino-6-methoxy-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867215-32-5P, 1-Ethylamino-6-methoxy-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867215-33-6P, 6-Methoxy-1-(morpholin-4-yl)-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867215-34-7P, 1-Benzylamino-6-methoxy-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867215-35-8P, 1-Cyclohexylamino-6-methoxy-3-phenyl-1H-indene-2-carboxylic acid ethyl ester
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of indenes as selective modulators of peroxisome proliferator activated receptors)

IT 9004-10-8, Insulin, biological studies
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(hyperinsulinemia; preparation of indenes as selective modulators of peroxisome proliferator activated receptors)

IT 94-02-0, Ethyl benzoylacetate 100-46-9, Benzylamine, reactions 100-52-7, Benzaldehyde, reactions 100-59-4, Phenylmagnesium chloride 103-74-2, 2-Pyridineethanol 105-58-8, Diethyl carbonate 108-91-8, Cyclohexylamine, reactions 109-89-7, Diethylamine, reactions 110-91-8, Morpholine, reactions 585-74-0 622-40-2, 4-(2-Hydroxyethyl)morpholine 637-59-2, 1-Bromo-3-phenylpropane 824-98-6, 3-Methoxybenzyl chloride 931-51-1, Cyclohexylmagnesium chloride 1068-55-9, Isopropylmagnesium chloride 6921-34-2, Benzylmagnesium chloride 36282-40-3,

3-Methoxyphenylmagnesium bromide 60760-06-7, 3-Chloromethylphenol 867187-77-7, 3-Phenyl-1-[3-(3-phenylpropoxy)phenyl]-2-propen-1-one
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of indenes as selective modulators of peroxisome proliferator activated receptors)

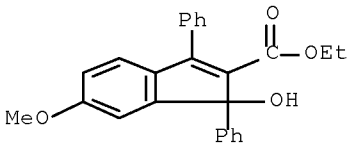
IT 33166-79-9P, 3-Oxo-3-(m-tolyl)propionic acid ethyl ester 850209-49-3P, 6-Methoxy-1-oxo-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867187-56-2P, 2-(3-Hydroxybenzyl)-3-oxo-3-phenylpropionic acid ethyl ester 867187-57-3P, 6-Hydroxy-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867187-58-4P, 6-Hydroxy-1-oxo-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867187-59-5P, 1-Oxo-3-phenyl-6-(3-phenylpropoxy)-1H-indene-2-carboxylic acid ethyl ester 867187-60-8P, 1-Hydroxyimino-3-phenyl-6-(3-phenylpropoxy)-1H-indene-2-carboxylic acid ethyl ester 867187-62-0P, 6-[2-(Morpholin-4-yl)ethoxy]-1-oxo-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867187-79-9P, 1-Oxo-3-phenyl-6-(3-phenylpropoxy)-1H-indene-2-carbonitrile 867187-84-6P, 2-(3-Methylbenzoyl)-3-phenylacrylic acid ethyl ester 867187-85-7P, 5-Methyl-3-oxo-1-phenylindane-2-carboxylic acid ethyl ester 867187-86-8P, 6-Methyl-1-oxo-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867187-87-9P, 6-Bromomethyl-1-oxo-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867187-88-0P, 6-[(Morpholin-4-yl)methyl]-1-oxo-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867187-90-4P, 1-Oxo-3-phenyl-6-(3-phenylpropoxy)-1H-indene-2-carboxylic acid methyl ester 867214-90-2P, 6-Methoxy-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867214-92-4P, 2-(3-Methoxybenzyl)-3-oxo-3-phenylpropionic acid ethyl ester 867215-03-0P, 6-[2-(Pyridin-2-yl)ethoxy]-1-oxo-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867215-05-2P, 3-Phenyl-6-(3-phenylpropoxy)inden-1-one 867215-06-3P, 2-Bromo-3-phenyl-6-(3-phenylpropoxy)inden-1-one 867215-14-3P, 1-Bromo-6-methoxy-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867215-17-6P, 1-Hydroxyimino-6-methoxy-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867215-20-1P, 6-Hydroxy-1-oxo-3-phenyl-1H-indene-2-carboxylic acid methyl ester 867215-21-2P, 6-Hydroxy-1-oxo-3-phenyl-1H-indene-2-carboxylic acid 867215-22-3P, 6-Hydroxy-1-oxo-3-phenyl-1H-indene-2-carboxylic acid cyclohexylamide 867215-23-4P, 6-[2-(Morpholin-4-yl)ethoxy]-1-oxo-3-phenyl-1H-indene-2-carboxylic acid cyclohexylamide 867215-24-5P, 1-Hydroxyimino-6-[2-(morpholin-4-yl)ethoxy]-3-phenyl-1H-indene-2-carboxylic acid cyclohexylamide 867215-26-7P, 1-Hydroxyimino-3-phenyl-6-(3-phenylpropoxy)-1H-indene-2-carbonitrile
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of indenes as selective modulators of peroxisome proliferator activated receptors)

IT 50-99-7, D-Glucose, biological studies
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(reducers of blood glucose levels; preparation of indenes as selective modulators of peroxisome proliferator activated receptors)

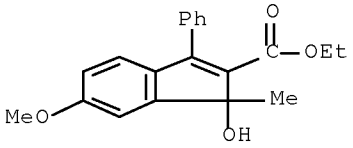
IT 867214-93-5P, 1-Hydroxy-6-methoxy-1,3-diphenyl-1H-indene-2-carboxylic acid ethyl ester 867214-96-8P, 1-Hydroxy-6-methoxy-1-methyl-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867214-97-9P, 1-Benzyl-1-hydroxy-6-methoxy-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867214-98-0P, 1-Cyclohexyl-1-hydroxy-6-methoxy-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867214-99-1P, 1-Hydroxy-1,3-diphenyl-6-(3-phenylpropoxy)-1H-indene-2-carboxylic acid ethyl ester 867215-16-5P, 1-Amino-6-methoxy-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867215-18-7P, 1-Amino-3-phenyl-6-(3-phenylpropoxy)-1H-indene-2-carboxylic acid ethyl ester 867215-19-8P, 1-Amino-6-[2-(morpholin-4-yl)ethoxy]-3-phenyl-1H-indene-2-carboxylic acid cyclohexylamide
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic

preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(drug candidate; preparation of indenes as selective modulators of peroxisome proliferator activated receptors)

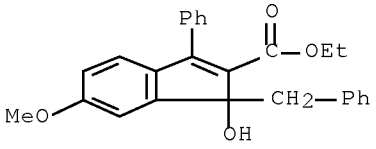
RN 867214-93-5 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-hydroxy-6-methoxy-1,3-diphenyl-, ethyl ester (CA INDEX NAME)



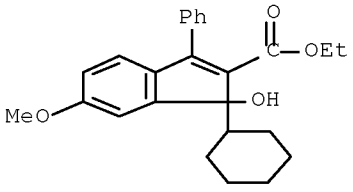
RN 867214-96-8 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-hydroxy-6-methoxy-1-methyl-3-phenyl-, ethyl ester (CA INDEX NAME)



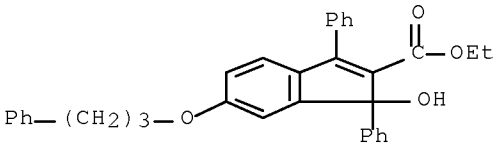
RN 867214-97-9 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-hydroxy-6-methoxy-3-phenyl-1-(phenylmethyl)-, ethyl ester (CA INDEX NAME)



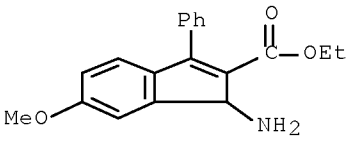
RN 867214-98-0 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-cyclohexyl-1-hydroxy-6-methoxy-3-phenyl-, ethyl ester (CA INDEX NAME)



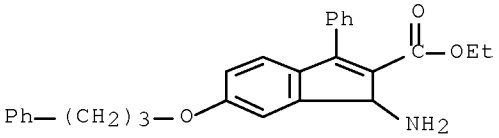
RN 867214-99-1 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-hydroxy-1,3-diphenyl-6-(3-phenylpropoxy)-, ethyl ester (CA INDEX NAME)



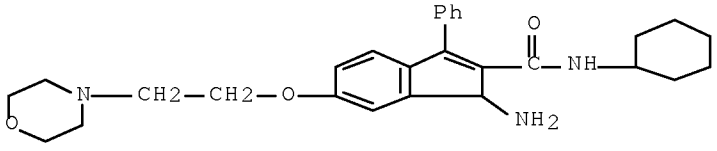
RN 867215-16-5 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-amino-6-methoxy-3-phenyl-, ethyl ester (CA INDEX NAME)



RN 867215-18-7 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-amino-3-phenyl-6-(3-phenylpropoxy)-, ethyl ester (CA INDEX NAME)



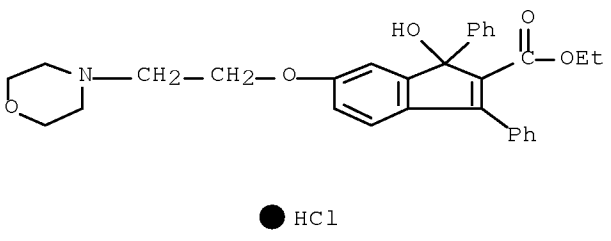
RN 867215-19-8 ZCAPLUS
CN 1H-Indene-2-carboxamide, 1-amino-N-cyclohexyl-6-[2-(4-morpholinyl)ethoxy]-3-phenyl- (CA INDEX NAME)



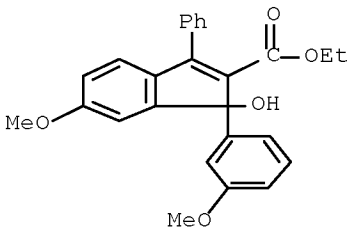
IT 867187-97-1P, 1-Hydroxy-6-[2-(morpholin-4-yl)ethoxy]-1,3-diphenyl-1H-indene-2-carboxylic acid ethyl ester hydrochloride 867214-94-6P, 1-Hydroxy-6-methoxy-1-(3-methoxyphenyl)-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867214-95-7P, 1-Hydroxy-1-isopropyl-6-methoxy-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867215-00-7P, 1-Hydroxy-6-[2-(morpholin-4-yl)ethoxy]-1,3-diphenyl-1H-indene-2-carboxylic acid ethyl ester 867215-01-8P, 1-Hydroxy-6-[(morpholin-4-yl)methyl]-1,3-diphenyl-1H-indene-2-carboxylic acid ethyl ester 867215-02-9P, 1-Hydroxy-1,3-diphenyl-6-[2-(pyridin-2-yl)ethoxy]-1H-indene-2-carboxylic acid ethyl ester 867215-04-1P, 1-Hydroxy-1,3-diphenyl-6-(3-phenylpropoxy)-1H-indene-2-carbonitrile 867215-07-4P, 1-Hydroxy-1,3-diphenyl-6-(3-phenylpropoxy)-1H-indene-2-carboxylic acid methyl ester 867215-08-5P, 1-Hydroxy-6-methoxy-1,3-diphenyl-1H-indene-2-carboxylic acid 867215-09-6P, 1-Hydroxy-6-methoxy-1-methyl-3-phenyl-1H-indene-2-carboxylic acid 867215-10-9P, 1-Benzyl-1-hydroxy-6-methoxy-3-phenyl-1H-indene-2-carboxylic acid 867215-11-0P, 1-Hydroxy-1,3-diphenyl-6-(3-phenylpropoxy)-1H-indene-2-carboxylic acid 867215-12-1P, 1-Cyclohexyl-1-hydroxy-6-methoxy-3-phenyl-1H-indene-2-carboxylic acid 867215-13-2P, 1,6-Dimethoxy-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867215-15-4P, 1-Ethoxy-6-methoxy-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867215-25-6P, 1-Amino-3-phenyl-6-(3-phenylpropoxy)-1H-indene-2-carbonitrile 867215-27-8P, 1-Acetylamino-6-methoxy-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867215-28-9P, 6-Methoxy-3-phenyl-1-propionylamino-1H-indene-2-carboxylic acid ethyl ester 867215-29-0P, 1-Acetylamino-3-phenyl-6-(3-phenylpropoxy)-1H-indene-2-carboxylic acid ethyl ester 867215-30-3P, 1-Acetylamino-6-[2-(morpholin-4-yl)ethoxy]-3-phenyl-1H-indene-2-carboxylic acid cyclohexylamide 867215-31-4P, 1-Diethylamino-6-methoxy-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867215-32-5P, 1-Ethylamino-6-methoxy-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867215-33-6P, 6-Methoxy-1-(morpholin-4-yl)-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867215-34-7P, 1-Benzylamino-6-methoxy-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867215-35-8P, 1-Cyclohexylamino-6-methoxy-3-phenyl-1H-indene-2-carboxylic acid ethyl ester
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of indenes as selective modulators of peroxisome proliferator activated receptors)

RN 867187-97-1 ZCAPLUS

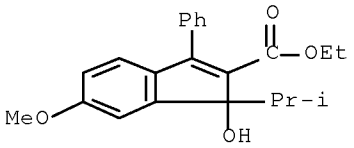
CN 1H-Indene-2-carboxylic acid, 1-hydroxy-6-[2-(4-morpholinyl)ethoxy]-1,3-diphenyl-, ethyl ester, hydrochloride (1:1) (CA INDEX NAME)



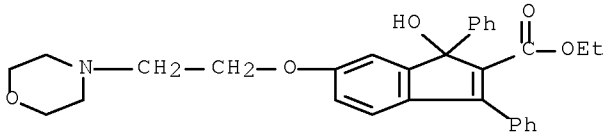
RN 867214-94-6 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-hydroxy-6-methoxy-1-(3-methoxyphenyl)-3-phenyl-, ethyl ester (CA INDEX NAME)



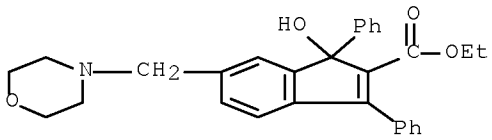
RN 867214-95-7 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-hydroxy-6-methoxy-1-(1-methylethyl)-3-phenyl-, ethyl ester (CA INDEX NAME)



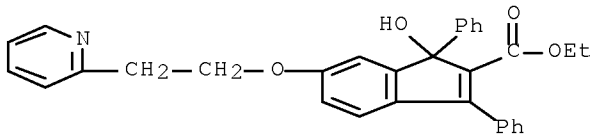
RN 867215-00-7 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-hydroxy-6-[2-(4-morpholinyl)ethoxy]-1,3-diphenyl-, ethyl ester (CA INDEX NAME)



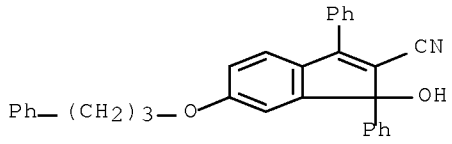
RN 867215-01-8 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-hydroxy-6-(4-morpholinylmethyl)-1,3-diphenyl-, ethyl ester (CA INDEX NAME)



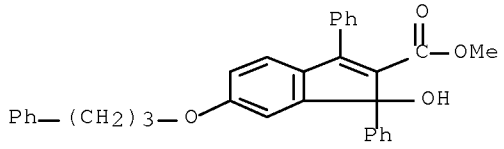
RN 867215-02-9 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-hydroxy-1,3-diphenyl-6-[2-(2-pyridinyl)ethoxy]-, ethyl ester (CA INDEX NAME)



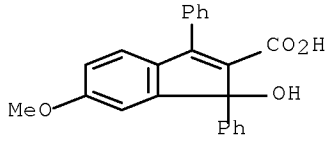
RN 867215-04-1 ZCAPLUS
CN 1H-Indene-2-carbonitrile, 1-hydroxy-1,3-diphenyl-6-(3-phenylpropoxy)- (CA INDEX NAME)



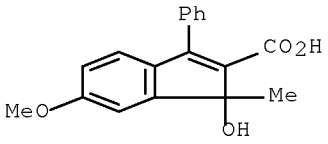
RN 867215-07-4 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-hydroxy-1,3-diphenyl-6-(3-phenylpropoxy)-, methyl ester (CA INDEX NAME)



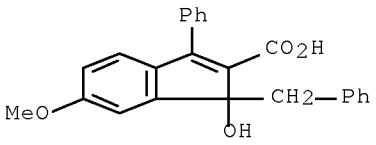
RN 867215-08-5 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-hydroxy-6-methoxy-1,3-diphenyl- (CA INDEX NAME)



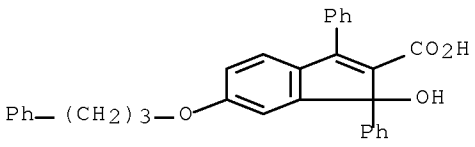
RN 867215-09-6 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-hydroxy-6-methoxy-1-methyl-3-phenyl- (CA INDEX NAME)



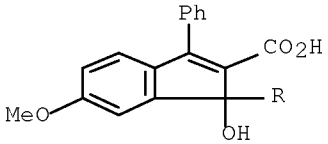
RN 867215-10-9 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-hydroxy-6-methoxy-3-phenyl-1-(phenylmethyl)- (CA INDEX NAME)

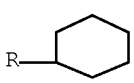


RN 867215-11-0 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-hydroxy-1,3-diphenyl-6-(3-phenylpropoxy)- (CA INDEX NAME)

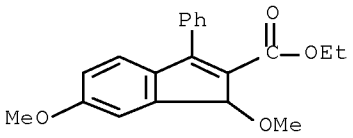


RN 867215-12-1 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-cyclohexyl-1-hydroxy-6-methoxy-3-phenyl- (CA INDEX NAME)

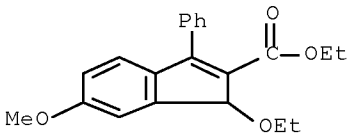




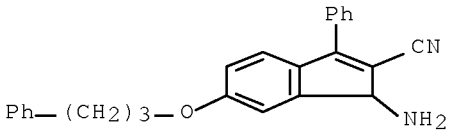
RN 867215-13-2 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1,6-dimethoxy-3-phenyl-, ethyl ester (CA INDEX NAME)



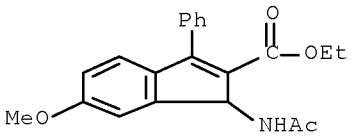
RN 867215-15-4 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-ethoxy-6-methoxy-3-phenyl-, ethyl ester (CA INDEX NAME)



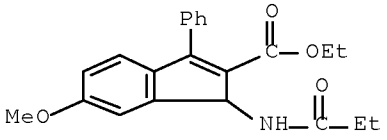
RN 867215-25-6 ZCAPLUS
CN 1H-Indene-2-carbonitrile, 1-amino-3-phenyl-6-(3-phenylpropoxy)- (CA INDEX NAME)



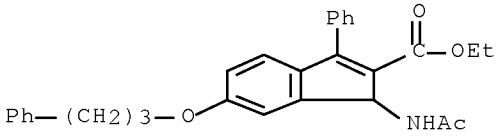
RN 867215-27-8 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-(acetylamino)-6-methoxy-3-phenyl-, ethyl ester (CA INDEX NAME)



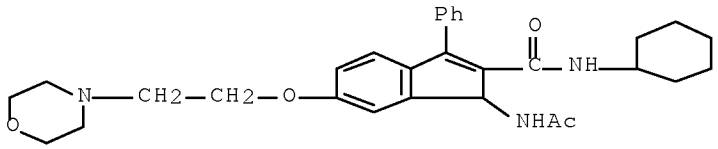
RN 867215-28-9 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 6-methoxy-1-[(1-oxopropyl)amino]-3-phenyl-, ethyl ester (CA INDEX NAME)



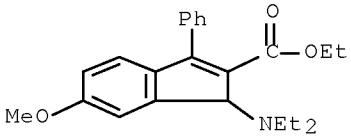
RN 867215-29-0 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-(acetylamino)-3-phenyl-6-(3-phenylpropoxy)-, ethyl ester (CA INDEX NAME)



RN 867215-30-3 ZCAPLUS
CN 1H-Indene-2-carboxamide, 1-(acetylamino)-N-cyclohexyl-6-[2-(4-morpholinyl)ethoxy]-3-phenyl- (CA INDEX NAME)

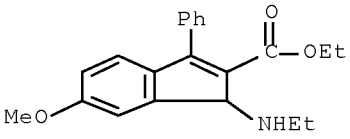


RN 867215-31-4 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-(diethylamino)-6-methoxy-3-phenyl-, ethyl ester (CA INDEX NAME)

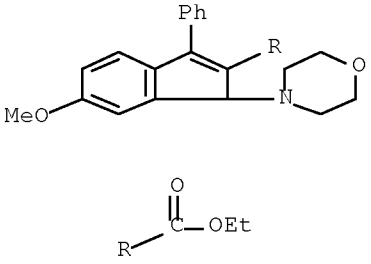


RN 867215-32-5 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-(ethylamino)-6-methoxy-3-phenyl-, ethyl

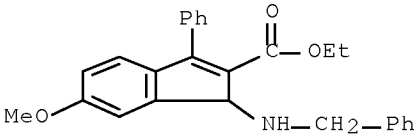
ester (CA INDEX NAME)



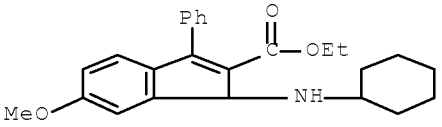
RN 867215-33-6 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 6-methoxy-1-(4-morpholinyl)-3-phenyl-, ethyl ester (CA INDEX NAME)



RN 867215-34-7 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 6-methoxy-3-phenyl-1-[(phenylmethyl)amino]-, ethyl ester (CA INDEX NAME)



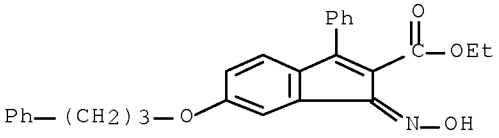
RN 867215-35-8 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-(cyclohexylamino)-6-methoxy-3-phenyl-, ethyl ester (CA INDEX NAME)



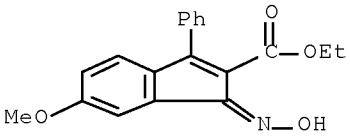
IT 867187-60-8P, 1-Hydroxyimino-3-phenyl-6-(3-phenylpropoxy)-1H-

indene-2-carboxylic acid ethyl ester 867215-17-6P, 1-Hydroxyimino-6-methoxy-3-phenyl-1H-indene-2-carboxylic acid ethyl ester 867215-24-5P, 1-Hydroxyimino-6-[2-(morpholin-4-yl)ethoxy]-3-phenyl-1H-indene-2-carboxylic acid cyclohexylamide 867215-26-7P, 1-Hydroxyimino-3-phenyl-6-(3-phenylpropoxy)-1H-indene-2-carbonitrile
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of indenes as selective modulators of peroxisome proliferator activated receptors)

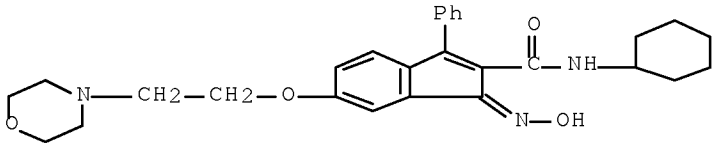
RN 867187-60-8 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-(hydroxyimino)-3-phenyl-6-(3-phenylpropoxy)-, ethyl ester (CA INDEX NAME)



RN 867215-17-6 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-(hydroxyimino)-6-methoxy-3-phenyl-, ethyl ester (CA INDEX NAME)



RN 867215-24-5 ZCAPLUS
CN 1H-Indene-2-carboxamide, N-cyclohexyl-1-(hydroxyimino)-6-[2-(4-morpholinyl)ethoxy]-3-phenyl- (CA INDEX NAME)



RN 867215-26-7 ZCAPLUS
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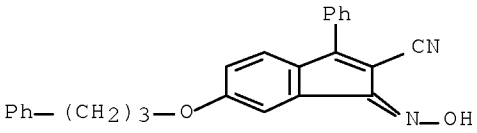

REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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STRUCTURE FILE UPDATES:   22 JUN 2008  HIGHEST RN 1029806-10-7
DICTIONARY FILE UPDATES:  22 JUN 2008  HIGHEST RN 1029806-10-7

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TSCA INFORMATION NOW CURRENT THROUGH January 9, 2008.

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experimental property data in the original document.  For information
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Uploading L5.str
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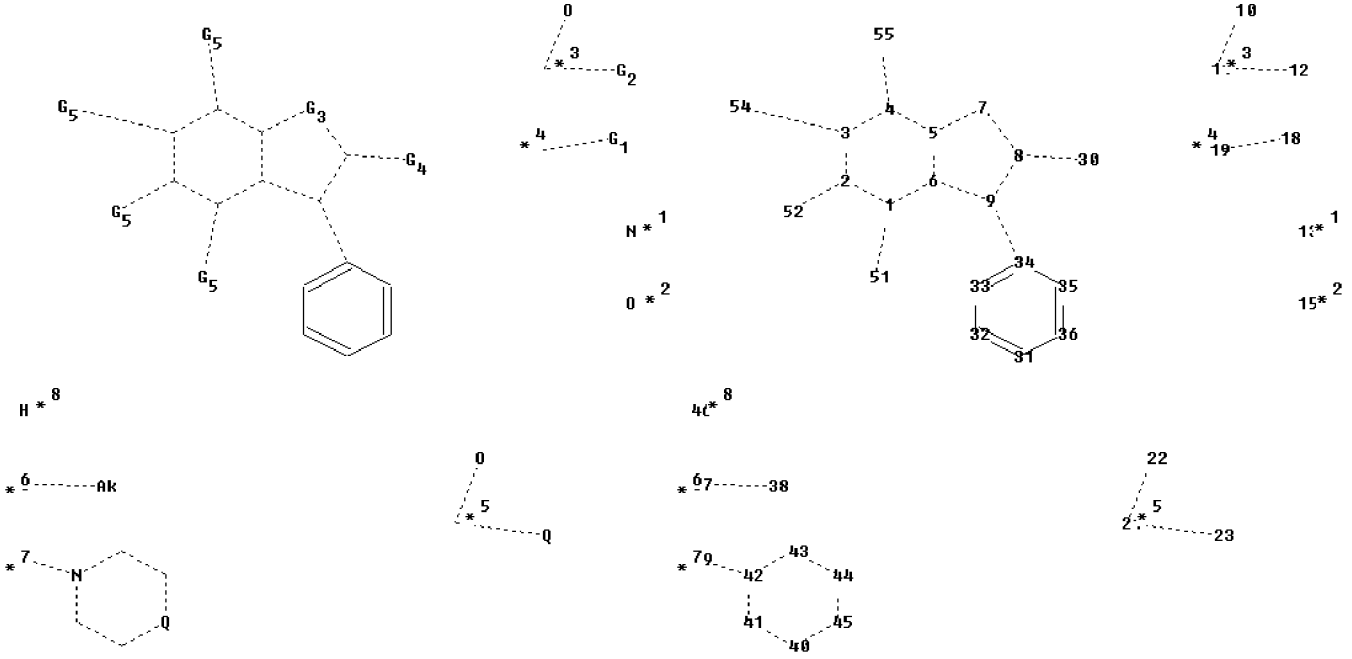

```
chain nodes :
10  12  15  18  21  22  23  30  37  38  39  46  51  52  54  55
ring nodes :
1  2  3  4  5  6  7  8  9  11  19  31  32  33  34  35  36  40  41  42  43  44  45

ring/chain nodes :
13
```

```
chain bonds :
1-51  2-52  3-54  4-55  8-30  9-34  10-11  11-12  18-19  21-22  21-23  37-38  39-42

ring bonds :
1-2  1-6  2-3  3-4  4-5  5-6  5-7  6-9  7-8  8-9  31-32  31-36  32-33  33-34  34-35
35-36  40-41  40-45  41-42  42-43  43-44  44-45
exact/norm bonds :
1-2  1-6  1-51  2-3  2-52  3-4  3-54  4-5  4-55  5-6  5-7  6-9  7-8  8-9  8-30  9-
34
10-11  11-12  18-19  21-22  21-23  37-38  39-42  40-41  40-45  41-42  42-43  43-44
44-45
normalized bonds :
31-32  31-36  32-33  33-34  34-35  35-36


G1:[*1],[*2]

G2:Cb,Ak

G3:[*3],[*4]

G4:CN,[*5]

G5:[*6],[*7],[*8]

Connectivity :
21:3 E exact RC ring/chain  22:1 E exact RC ring/chain
Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  7:Atom  8:Atom  9:Atom  10:CLASS
11:Atom  12:CLASS  13:CLASS  15:CLASS  18:CLASS  19:Atom  21:CLASS  22:CLASS
23:CLASS  30:CLASS
31:Atom  32:Atom  33:Atom  34:Atom  35:Atom  36:Atom  37:CLASS  38:CLASS  39:CLASS
40:Atom  41:Atom
42:Atom  43:Atom  44:Atom  45:Atom  46:CLASS  51:CLASS  52:CLASS  54:CLASS
55:CLASS



Uploading L43.str
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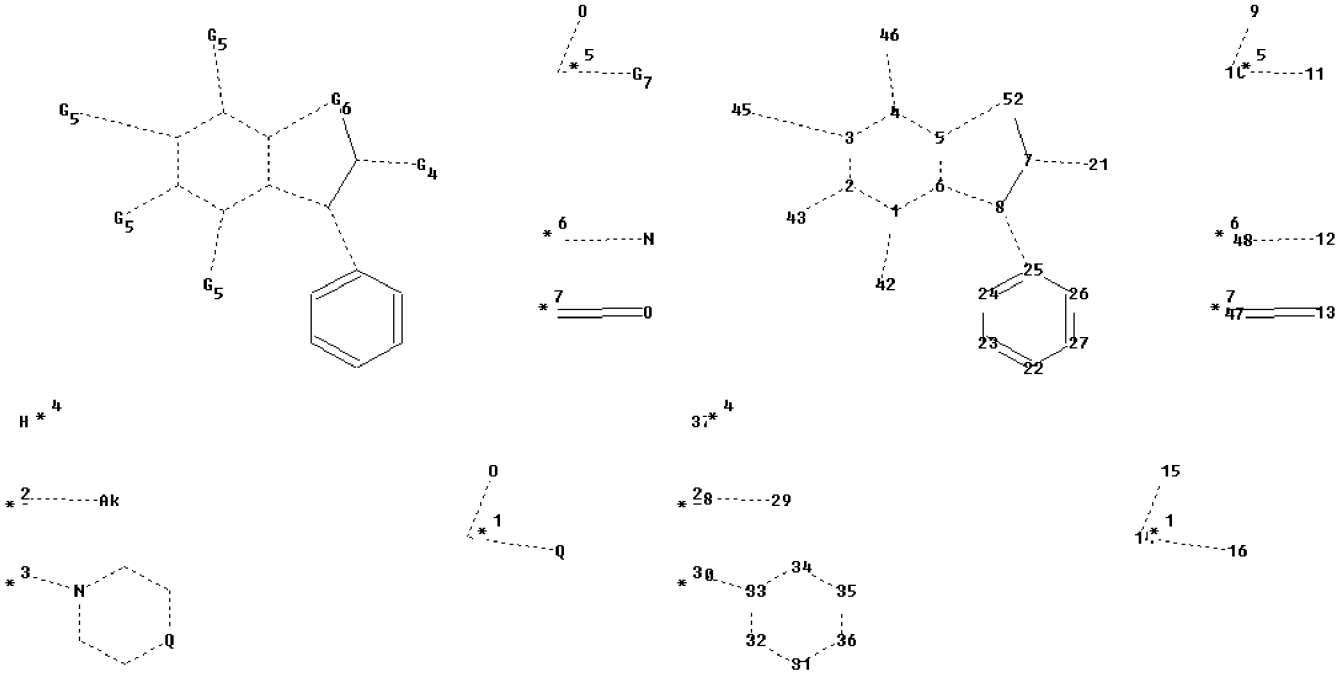

chain nodes :
9 11 13 14 15 16 21 28 29 30 37 42 43 45 46
ring nodes :
1 2 3 4 5 6 7 8 10 22 23 24 25 26 27 31 32 33 34 35 36 47 48 52
ring/chain nodes :
12
chain bonds :
1-42 2-43 3-45 4-46 7-21 8-25 9-10 10-11 12-48 13-47 14-15 14-16 28-29 30-33
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-52 6-8 7-8 7-52 22-23 22-27 23-24 24-25 25-26
26-27 31-32 31-36 32-33 33-34 34-35 35-36
exact/norm bonds :
1-2 1-6 1-42 2-3 2-43 3-4 3-45 4-5 4-46 5-6 5-52 6-8 7-21 7-8 7-52 8-25 9-10 10-11 12-48 13-47 14-15 14-16 28-29 30-33 31-32 31-36 32-33 33-34 34-35 35-36

normalized bonds :
22-23 22-27 23-24 24-25 25-26 26-27

G4:CN,[*1]

G5:[*2],[*3],[*4]

G6:[*5],[*6],[*7]

G7:Cb,Ak

Connectivity :
7:3 E exact RC ring/chain 8:3 E exact RC ring/chain 14:3 E exact RC ring/chain 15:1 E exact RC ring/chain 47:3 E exact RC ring/chain 48:3 E exact RC ring/chain
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:CLASS 10:Atom

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11:CLASS  12:CLASS  13:CLASS  14:CLASS  15:CLASS  16:CLASS  21:CLASS  22:Atom
23:Atom  24:Atom  25:Atom
26:Atom  27:Atom  28:CLASS  29:CLASS  30:CLASS  31:Atom  32:Atom  33:Atom  34:Atom
35:Atom
36:Atom  37:CLASS  42:CLASS  43:CLASS  45:CLASS  46:CLASS  47:CLASS  48:CLASS
52:CLASS



=> file zcaplus
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FILE LAST UPDATED: 22 Jun 2008  (20080622/ED)

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  This file contains CAS Registry Numbers for easy and accurate
  substance identification.
'OBI' IS DEFAULT SEARCH FIELD FOR 'ZCAPLUS' FILE

=> d stat que L47
L5              STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -  AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.
L7          427 SEA FILE=REGISTRY SSS FUL L5
L43             STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -  AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.
L45          55 SEA FILE=REGISTRY SUB=L7 SSS FUL L43
L47          35 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  L45


=> d stat que L82
L5              STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -  AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.
L7          427 SEA FILE=REGISTRY SSS FUL L5
L43             STR
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* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -  AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.
L45          55 SEA FILE=REGISTRY SUB=L7 SSS FUL L43
L47          35 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  L45
L54      171149 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  ?DIABET?/BI
L55       56841 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  OBES?/BI
L56       11261 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  ANTIOBES?/BI
L57      289180 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  ?ARTER?/BI
L58      504356 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  ?LIPID?/BI
L59      225556 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  ?INSULIN?/BI
L60      124786 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  ?HYPERTENS?/BI
L61       32726 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  ?HYPOTENS?/BI
L62       89940 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  ?OSTEO?/BI
L63      594903 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  LIVER/BI
L64       25633 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  ?CIRRHOS?/BI
L65       45105 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  ?ASTHMA?/BI
L66      553816 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  ?NEOPLAS?/BI
L67      407468 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  ?CANCER?/BI
L68      662469 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  ?TUMOR?/BI
L69        5585 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  ?TUMOUR?/BI
L70       56405 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  ?SARCOMA?/BI
L71      123066 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  ?LEUKEM?/BI
L72        1597 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  ?LEUKAEM?/BI
L73      308147 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  ?CARCINO?/BI
L74       44793 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  ?LYMPHOM?/BI
L75       39743 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  ?MELANOM?/BI
L76       51481 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  ?ANGIOGEN?/BI
L78       11482 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  PPAR/BI
L79       23760 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  PEROXISOM?/BI
L82           8 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  L47 AND (L54 OR L55 OR L56 OR
                L57 OR L58 OR L59 OR L60 OR L61 OR L62 OR L63 OR L64 OR L65 OR
                L66 OR L67 OR L68 OR L69 OR L70 OR L71 OR L72 OR L73 OR L74 OR
                L75 OR L76 OR L78 OR L79)


=> s L47,L82 not L101,L102,L28,L42,L81
L108        21 (L47 OR L82) NOT (L101 OR L102 OR L28 OR L42 OR L81)

=> d ibib abs hitind hitstr L108 1-21

L108 ANSWER 1 OF 21  ZCAPLUS  COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER:         2007:1474750  ZCAPLUS  Full-text
DOCUMENT NUMBER:          148:284803
TITLE:                    Polarizing the Nazarov Cyclization: The Impact of
                          Dienone Substitution Pattern on Reactivity and
                          Selectivity
AUTHOR(S):                He, Wei; Herrick, Ildiko R.; Atesin, Tulay A.;
                          Caruana, Patrick A.; Kellenberger, Colleen A.;
                          Frontier, Alison J.
CORPORATE SOURCE:         Department of Chemistry, University of Rochester,
                          Rochester, NY, 14627, USA
SOURCE:                   Journal of the American Chemical Society (2008),
                          130(3), 1003-1011
                          CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER:                American Chemical Society
DOCUMENT TYPE:            Journal
LANGUAGE:                 English
OTHER SOURCE(S):          CASREACT 148:284803
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AB The impact of dienone substitution on the Nazarov cyclization has been examined in detail. Substrates R1R2C:CR3C(O)CR4:CHR5 [R1 = R2 = H, R3 = Me; R1R3 = (CH2)3O, R2 = H; R1R3 = (CH2)4, R2 = H, Me; R1R2C:CR3 = 3,5-bis(triisopropylsilyloxy)phenyl, etc.; R4 = MeO2C, Me2NCO, 4-MeC6H4SO2, (EtO)2PO, etc.; R5 = n-Pr, Ph, 4-MeOC6H4, 2,4,6-(MeO)3C6H2, PhCH:CH, etc.], bearing different substituents at each of four positions on the dienone backbone, were systematically probed in order to identify trends leading to higher reactivity and better selectivity. Desymmetrization of the pentadienyl cation and oxyallyl cation intermediates through placement of polarizing groups at both the C-2 and C-4 positions was found to be particularly effective. These modifications allowed cyclizations to occur in the presence of catalytic amts. of mild Lewis acids. It was also found that stereoconvergent cyclization of mixts. of E and Z isomers of alkylidene β-ketoesters occurred via an efficient isomerization process that occurred under the reaction conditions.

CC 24-4 (Alicyclic Compounds)

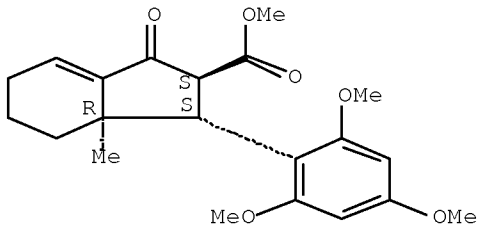
IT 638186-65-9P 638186-66-0P 638186-67-1P 638186-68-2P 638186-69-3P
638186-76-2P 638186-78-4P 638186-79-5P 638186-81-9P
638186-85-3P 638186-91-1P 638186-92-2P 879048-60-9P
1007841-69-1P 1007841-71-5P 1007841-82-8P 1007841-90-8P
1007841-92-0P 1007841-93-1P 1007841-94-2P
1007841-95-3P 1007841-97-5P 1007842-03-6P 1007842-04-7P
1007842-05-8P 1007842-06-9P 1007842-07-0P 1007842-08-1P
1007842-09-2P 1007842-10-5P 1007842-22-9P 1007842-23-0P
1007842-24-1P 1007842-25-2P 1007842-26-3P 1007842-28-5P
1007842-30-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(impact of the dienone substitution pattern on reactivity and selectivity of Nazarov cyclization)

IT 638186-79-5P 638186-91-1P 1007841-69-1P
1007841-92-0P 1007841-93-1P 1007841-94-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(impact of the dienone substitution pattern on reactivity and selectivity of Nazarov cyclization)

RN 638186-79-5 ZCAPLUS

CN 1H-Indene-2-carboxylic acid, 2,3,3a,4,5,6-hexahydro-3a-methyl-1-oxo-3-(2,4,6-trimethoxyphenyl)-, methyl ester, (2R,3R,3aS)-rel- (CA INDEX NAME)

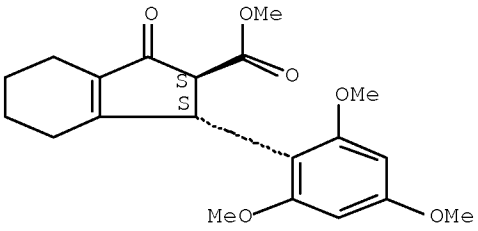
Relative stereochemistry.



RN 638186-91-1 ZCAPLUS

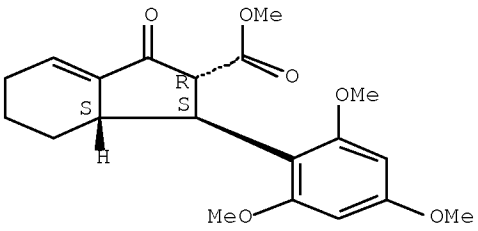
CN 1H-Indene-2-carboxylic acid, 2,3,4,5,6,7-hexahydro-1-oxo-3-(2,4,6-trimethoxyphenyl)-, methyl ester, (2R,3R)-rel- (CA INDEX NAME)

Relative stereochemistry.



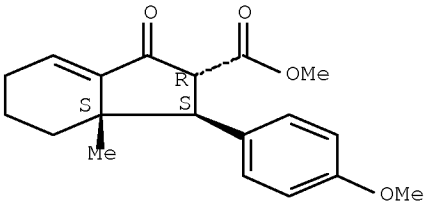
RN 1007841-69-1 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 2,3,3a,4,5,6-hexahydro-1-oxo-3-(2,4,6-trimethoxyphenyl)-, methyl ester, (2R,3S,3aS)-rel- (CA INDEX NAME)

Relative stereochemistry.



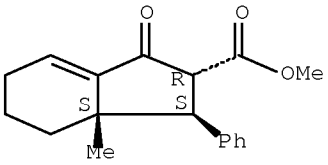
RN 1007841-92-0 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 2,3,3a,4,5,6-hexahydro-3-(4-methoxyphenyl)-3a-methyl-1-oxo-, methyl ester, (2R,3S,3aS)-rel- (CA INDEX NAME)

Relative stereochemistry.



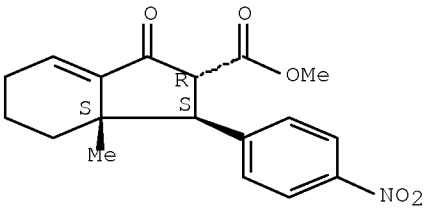
RN 1007841-93-1 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 2,3,3a,4,5,6-hexahydro-3a-methyl-1-oxo-3-phenyl-, methyl ester, (2R,3S,3aS)-rel- (CA INDEX NAME)

Relative stereochemistry.



RN 1007841-94-2 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 2,3,3a,4,5,6-hexahydro-3a-methyl-3-(4-nitrophenyl)-1-oxo-, methyl ester, (2R,3S,3aS)-rel- (CA INDEX NAME)

Relative stereochemistry.



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L108 ANSWER 2 OF 21 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2007:706387 ZCAPLUS Full-text
DOCUMENT NUMBER: 147:118039
TITLE: Preparation of indanes as modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents
INVENTOR(S): Duan, Jingwu; Jiang, Bin
PATENT ASSIGNEE(S): Bristol-Myers Squibb Company, USA
SOURCE: PCT Int. Appl., 175 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

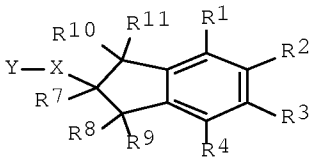
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2007073503	A2	20070628	WO 2006-US49075	20061221
WO 2007073503	A3	20071108		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ,

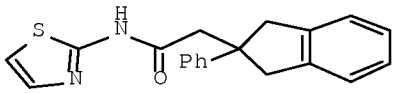
CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AP, EA, EP, OA

US 20070185056 A1 20070809 US 2006-642508 20061220
PRIORITY APPLN. INFO.: US 2005-752353P P 20051221
US 2006-642508 A 20061220
OTHER SOURCE(S): MARPAT 147:118039

GI



I



II

AB Indanes I [A1, A2 = bond, C1-3 alkanediyl, C1-3 alkenediyl; Q = bond, carbonyl, oxycarbonyl, (un)substituted carbonylamino, sulfonylamino, etc.; R1, R2, R3, R4 = H, halo, alkyl, (un)substituted alkenyl or alkynyl, azido, nitro, cyano, (un)substituted alkoxy or aryloxy; R1R2, R2R3 or R3R4 may also be joined to form a ring; R7, R8, R9, R10, R11 = H, halogen, (un)substituted alkyl, alkenyl or alkynyl, nitro, cyano, (un)substituted alkoxy or aryloxy, etc.; X = A1QA2; Y = H, (un)substituted alkyl, aryl, heteroaryl, heterocyclyl, alkoxy, or aryloxy such that if X = (un)substituted aminocarbonyl, Y ≠ pyridinyl, pyrimidinyl, oxopyridinyl, or arylpyrazolyl] such as indaneacetamide II, are prepared as potential modulators of glucocorticoid receptors, NF-κB, or AP-1 activity for use as potential antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents. Alkylation of 2-phenyl-1,3-indanedione with tert-Bu bromoacetate, acid hydrolysis of the tert-Bu ester, palladium-catalyzed reduction of the dioxoindaneacetic acid to an indaneacetic acid, and coupling of the indaneacetic acid with 2-aminothiazole provides II. Preparative data for the example compds. are given. No biol. activities are reported for the example compds.

IC ICM A61K

CC 25-19 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
Section cross-reference(s): 1, 63

ST indane prepn modulator glucocorticoid receptor NFkB AP1 activity; potential antiobesity antidiabetic antiinflammatory immunomodulatory activity indane

IT Transcription factors
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(AP-2 (activator protein 2); preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents and their use in concert with other agents)

IT Inflammatory bowel disease
(Crohn's disease; preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents)

IT Nervous system, disease
(Guillain-Barre syndrome; preparation of indanes as potential modulators of

glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents)

IT Histocompatibility antigens
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(HLA_DP4; preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents)

IT Proteins
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(MTP (microsomal triglyceride-exchanging protein); preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents and their use in concert with other agents)

IT Sodium-dependent glucose transporters
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(SGLT2, inhibitors, codrugs; preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents)

IT Inflammation
Pancreas, disease
(acute pancreatitis; preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents)

IT Myocarditis
(acute rheumo-; preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents)

IT Gout
Respiratory distress syndrome
(acute; preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents)

IT Allergy
Eye, disease
Inflammation
(allergic conjunctivitis; preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents)

IT Allergy
(allergic dermatitis; preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents)

IT Allergy
Inflammation
Nose, disease
(allergic rhinitis, perennial; preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents)

IT Allergy

Inflammation
Nose, disease
(allergic rhinitis, seasonal; preparation of indanes as potential modulators
of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents)

IT Allergy
Inflammation
Nose, disease
(allergic rhinitis; preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents)

IT Dermatitis
(allergic; preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents)

IT Respiratory system, disease
(allergy; preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents)

IT Transplant and Transplantation
(allotransplant, skin; preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents)

IT Skin
(allotransplant; preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents)

IT Lung, disease
(alveolitis; preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents)

IT Inflammation
Spinal column, disease
(ankylosing spondylitis; preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents)

IT Cytotoxic agents
(anti-vascular hyperproliferation agents, codrugs; preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents)

IT Alopecia
(areata; preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents)

IT Dermatitis
(atopic; preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents)

IT Anemia (disease)

Autoimmune disease
(autoimmune hemolytic anemia; preparation of indanes as potential modulators
of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents)

IT Autoimmune disease
Inflammation
Thyroid gland, disease
(autoimmune thyroiditis; preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents)

IT Alopecia
Vasculitis
(autoimmune; preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents)

IT Transplant and Transplantation
(bone marrow; preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents)

IT Joint, anatomical
(bursa, disease, acute bursitis; preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents)

IT Joint, anatomical
(bursa, disease, subacute bursitis; preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents)

IT Tuberculostatics
(chemotherapy; preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents)

IT Development, mammalian postnatal
(child; preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents)

IT Eye, disease
(chorio-retinitis; preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents)

IT Lung, disease
(chronic obstructive pulmonary disease; preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents)

IT Inflammation
Pancreas, disease
(chronic pancreatitis; preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or

immunomodulatory agents)
IT Sulfonylureas
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(codrug; preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents and their use in concert with other agents)
IT 5-HT reuptake inhibitors
Angiotensin receptor antagonists
Antibiotics
Antidepressants
Antidiabetic agents
Antihypertensives
Antiobesity agents
Antiosteoporotic agents
Antiviral agents
Appetite depressants
Calcium channel blockers
Fungicides
Hypolipemic agents
Immunosuppressants
Platelet aggregation inhibitors
β3-Adrenoceptor agonists
(codrugs; preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents and their use in concert with other agents)
IT Adrenal cortex, disease
(congenital adrenal hyperplasia; preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents)
IT Hyperplasia
(congenital adrenal; preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents)
IT Dermatitis
(contact; preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents)
IT Eye
(cornea, transplant; preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents)
IT Transplant and Transplantation
(cornea; preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents)
IT Allergy
(delayed hypersensitivity; preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents)
IT Tendon
(disease, tenosynovitis, acute non-specific; preparation of indanes as

potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents)

IT Platelet (blood)
(disease, thrombocytopenia, secondary, in adults; preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents)

IT Disease, animal
(epicondylitis; preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents)

IT Dermatitis
(exfoliative; preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents)

IT Tuberculosis
(fulminating or disseminated; preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents)

IT Inflammation
Kidney, disease
(glomerulonephritis; preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents)

IT Transplant and Transplantation
(graft-vs.-host reaction; preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents)

IT Transplant and Transplantation
(heart; preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents)

IT Anemia (disease)
(hemolytic, acquired; preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents)

IT Anemia (disease)
(hemolytic, immuno-; preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents)

IT Eye, disease
(herpes zoster ophthalmicus; preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents)

IT Dermatitis
(herpetiformis, bullous; preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or

immunomodulatory agents)
IT Allergy
(hypersensitivity, to drugs; preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents)
IT Pituitary gland, disease
(hypopituitarism, autoimmune; preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents)
IT Adrenal gland, disease
(idiopathic adrenal insufficiency; preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents)
IT Purpura (disease)
(idiopathic thrombocytopenic, in adults; preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents)
IT Lymphoma
(in adults; preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents)
IT Autoimmune disease
(insulin-dependent diabetes mellitus; preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents)
IT Diabetes mellitus
(insulin-dependent; preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents)
IT Eye, disease
Inflammation
(iridocyclitis; preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents)
IT Eye, disease
Inflammation
(iritis; preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents)
IT Rheumatoid arthritis
(juvenile; preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents)
IT Eye, disease
Inflammation
(keratitis; preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity

, antidiabetic, antiinflammatory, or immunomodulatory agents)
IT Transplant and Transplantation
(kidney; preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents)
IT Mouth, disease
Skin, disease
(lichen planus; preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents)
IT Transplant and Transplantation
(liver; preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents)
IT Transplant and Transplantation
(lung; preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents)
IT Disease, animal
(morphea; preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents)
IT Erythema
(multiforme, severe; preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents)
IT Diabetes mellitus
(non-insulin-dependent; preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents)
IT Leukemia
(of childhood; preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents)
IT Inflammation
Nerve, disease
(optic neuritis; preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents)
IT Transplant and Transplantation
(pancreas; preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents)
IT Skin, disease
(pemphigus; preparation of indanes as potential modulators of glucocorticoid
receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents)
IT Anemia (disease)
(pernicious anemia; preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or

immunomodulatory agents)
IT Inflammation
Lung, disease
(pneumonitis; preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents)
IT Autoimmune disease
Endocrine system, disease
(polyglandular syndrome; preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents)
IT Osteoarthritis
(post-traumatic; preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents)
IT Addison's disease
Anti-inflammatory agents
Antiarthritics
Antirheumatic agents
Asthma
Atherosclerosis
Autoimmune disease
Behcet's syndrome
Celiac disease
Coronary restenosis
Dermatitis
Dermatomyositis
Eczema
Graves' disease
Hay fever
Hepatitis
Human
Inflammation
Inflammatory bowel disease
Leukemia
Multiple sclerosis
Myasthenia gravis
Obesity
Osteoarthritis
Pharmaceutical carriers
Psoriasis
Rheumatoid arthritis
Scleroderma
Seborrhea
Sepsis
Sezary syndrome
Sjogren syndrome
Stenosis
Transplant rejection
Urticaria
Uveitis
Vascular restenosis
Vitiligo
(preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents)

IT Allergy inhibitors
Antiasthmatics
Antidiabetic agents
Antitumor agents
Bronchodilators
Combination chemotherapy
Nervous system agents
(preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents and their use in concert with other agents)

IT Interleukin 2
Low-density lipoprotein receptors
Thyroid hormone receptors
β3-Adrenoceptors
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents and their use in concert with other agents)

IT Arthritis
(psoriatic arthritis; preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents)

IT Inflammation
(pulmonary alveolitis; preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents)

IT Skin, disease
(pyoderma, pyoderma gangrenum; preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents)

IT Allergy
(respiratory tract; preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents)

IT Disease, animal
(serum sickness; preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents)

IT Transplant and Transplantation
(small intestine; preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents)

IT Sarcoidosis
(symptomatic; preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents)

IT Osteoarthritis
(synovitis of; preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as

antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents)
IT Lupus erythematosus
(systemic; preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents)
IT Inflammation
(tenosynovitis, acute non-specific; preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents)
IT Blood, disease
(thrombocytopenia, secondary, in adults; preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents)
IT Inflammation
Thyroid gland, disease
(thyroiditis, non-suppurative; preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents)
IT Bone marrow
Heart
Kidney
Liver
Lung
Pancreas
Small intestine
(transplant; preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents)
IT Inflammatory bowel disease
(ulcerative colitis; preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents)
IT Colitis
(ulcerative; preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents)
IT Heart valve
(xenograft; preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents)
IT Peroxisome proliferator-activated receptors
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(α; preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents and their use in concert with other agents)
IT Interferons
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(β, codrug; preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents and their use in concert with other agents)

IT Peroxisome proliferator-activated receptors
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(γ; preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents and their use in concert with other agents)

IT 137862-53-4, Valsartan
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(codrug; preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents)

IT 50-02-2, Dexamethasone 50-18-0, Cyclophosphamide 50-23-7, Hydrocortisone 50-78-2, Aspirin 51-21-8, 5-Fluorouracil 51-64-9, Dexamphetamine 52-24-4, Thiotepa 52-53-9, Verapamil 53-03-2, Prednisone 53-86-1, Indomethacin 56-03-1, Biguanide 58-32-2, Dipyridamole 59-05-2, Methotrexate 59-67-6, Niacin, biological studies 67-78-7, Triamcinolone diacetate 94-20-2, Chloropropamide 122-09-8, Phentermine 446-86-6, Azathioprine 525-66-6, Propranolol 637-07-0, Clofibrate 657-24-9, Metformin 4205-91-8, Clonidine hydrochloride 5536-17-4, Vidarabine 10238-21-8, Glyburide 14838-15-4, Phenylpropanolamine 15307-79-6, Diclofenac sodium 15663-27-1, Cisplatin 15687-27-1, Ibuprofen 19237-84-4, Prazosin hydrochloride 21187-98-4, Gliclazide 21829-25-4, Nifedipine 22071-15-4, Ketoprofen 22204-53-1, Naproxen 22232-71-9 25812-30-0, Gemfibrozil 29094-61-9, Glipizide 36322-90-4, Piroxicam 41575-94-4, Carboplatin 42200-33-9, Nadolol 49562-28-9, Fenofibrate 54870-28-9, Meglitinide 55142-85-3, Ticlopidine 56180-94-0, Acarbose 59277-89-3, Aciclovir 59865-13-3, Cyclosporin A 62571-86-2, Captopril 72432-03-2, Miglitol 72956-09-3, Carvedilol 75330-75-5, Lovastatin 75847-73-3, Enalapril 76547-98-3, Lisinopril 79902-63-9, Simvastatin 80830-42-8, Fentiapril 81093-37-0, Pravastatin 82410-32-0, Ganciclovir 85441-61-8, Quinapril 86541-75-5, Benazepril 87333-19-5, Ramipril 89149-10-0, Deoxyspergualin 89750-14-1, Glucagon-like peptide-1 93479-97-1, Glimepiride 93957-54-1, Fluvastatin 96829-58-2, Orlistat 97240-79-4, Topiramate 97322-87-7, Troglitazone 98048-97-6, Fosinopril 103775-10-6, Moexipril 104987-11-3, FK-506 105816-04-4, Nateglinide 106650-56-0, Sibutramine 111025-46-8, Pioglitazone 111470-99-6, Amlodipine besylate 113665-84-2, Clopidogrel 114798-26-4, Losartan 122320-73-4, Rosiglitazone 128794-94-5, Mycophenolate mofetil 134523-00-5, Atorvastatin 135062-02-1, Repaglinide 136470-78-5, Abacavir 138402-11-6, Irbesartan 141758-74-9, AC2993 143443-90-7, Ifetroban 144288-97-1, TS-962 145599-86-6, Cerivastatin 147511-69-1 159183-92-3, L750355 160135-92-2, Gemopatrilat 161600-01-7, Isaglitazone 162011-90-7, Rofecoxib 166518-60-1, Avasimibe 167305-00-2, Omapatrilat 169319-62-4, CGS 30440 169590-42-5, Celecoxib 170861-63-9, JTT-501 176435-10-2, LY315902 178759-95-0 182815-44-7, Cholestagel 196808-45-4, GI-262570 199113-98-9, NN-2344 199914-96-0, YM-440 213252-19-8, KRP297 244081-42-3, AJ9677 251572-86-8, P32/98 258345-41-4, GW-409544 282526-98-1 287714-41-4 335149-08-1, L 895645 335149-14-9, R 119702 335149-15-0, KAD 1129 335149-17-2, ARHO 39242 335149-23-0, NVP-DPP 728A 335149-25-2, CP 331648 430433-17-3, Glipyride 444069-80-1, Axokine 862273-00-5, Zidanocin
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(codrug; preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents and their use in concert with other agents)

IT 943-45-3D, derivs.
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(codrugs; preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents and their use in concert with other agents)

IT 7440-70-2, Calcium, biological studies
RL: ADV (Adverse effect, including toxicity); BSU (Biological study, unclassified); BIOL (Biological study)
(hypercalcemia cancer- associated; preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents)

IT 9001-62-1, Lipase 9015-82-1 9027-63-8, ACAT 9028-35-7 9029-60-1, Lipoxygenase 9033-06-1, Glucosidase 9077-14-9, Squalene synthetase 82707-54-8, Neutral endopeptidase
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(inhibitors, codrugs; preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents)

IT 943006-71-1P
RL: PAC (Pharmacological activity); PEP (Physical, engineering or chemical process); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); PROC (Process); RACT (Reactant or reagent); USES (Uses)
(preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents)

IT 943006-67-5P 943007-57-6P 943008-87-5P 943009-07-2P 943009-29-8P
RL: PAC (Pharmacological activity); PEP (Physical, engineering or chemical process); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)
(preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents)

IT 943006-68-6P 943006-69-7P 943006-72-2P 943006-73-3P 943007-58-7P 943007-59-8P 943009-43-6P 943009-45-8P
RL: PAC (Pharmacological activity); PUR (Purification or recovery); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents)

IT 943009-08-3P 943009-09-4P 943009-46-9P 943009-47-0P
RL: PAC (Pharmacological activity); PUR (Purification or recovery); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents)

IT 943006-52-8P 943006-54-0P 943006-66-4P 943006-76-6P 943006-77-7P 943006-81-3P 943006-82-4P 943006-88-0P 943006-95-9P 943006-99-3P 943007-02-1P 943007-06-5P 943007-09-8P 943007-12-3P 943007-24-7P

943007-29-2P 943007-35-0P 943007-39-4P 943007-41-8P 943007-43-0P
943007-45-2P 943007-46-3P 943007-50-9P 943007-51-0P 943007-60-1P
943007-70-3P 943007-71-4P 943007-77-0P 943008-22-8P 943008-39-7P
943008-45-5P 943008-53-5P 943008-54-6P 943008-57-9P 943008-58-0P
943008-61-5P 943008-64-8P 943008-65-9P 943008-74-0P 943008-75-1P
943008-82-0P 943008-83-1P 943008-88-6P 943008-89-7P 943008-91-1P
943009-34-5P 943009-35-6P 943009-36-7P 943009-37-8P 943009-38-9P
943009-49-2P 943010-14-8P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents)

IT 943006-49-3P 943006-50-6P 943006-51-7P 943006-53-9P 943006-55-1P
943006-56-2P 943006-57-3P 943006-58-4P 943006-59-5P 943006-60-8P
943006-61-9P 943006-62-0P 943006-63-1P 943006-64-2P 943006-65-3P
943006-70-0P 943006-74-4P 943006-75-5P 943006-78-8P 943006-79-9P
943006-80-2P 943006-83-5P 943006-84-6P 943006-85-7P 943006-86-8P
943006-90-4P 943006-92-6P 943006-94-8P 943006-97-1P 943007-01-0P
943007-04-3P 943007-07-6P 943007-10-1P 943007-14-5P 943007-16-7P
943007-18-9P 943007-20-3P 943007-22-5P 943007-27-0P 943007-31-6P
943007-33-8P 943007-37-2P 943007-42-9P 943007-44-1P 943007-47-4P
943007-48-5P 943007-49-6P 943007-52-1P 943007-53-2P 943007-54-3P
943007-55-4P 943007-56-5P 943007-61-2P 943007-62-3P 943007-63-4P
943007-64-5P 943007-65-6P 943007-66-7P 943007-67-8P 943007-68-9P
943007-69-0P 943007-72-5P 943007-73-6P 943007-74-7P 943007-75-8P
943007-76-9P 943007-78-1P 943007-79-2P 943007-80-5P 943007-81-6P
943007-82-7P 943007-83-8P 943007-84-9P 943007-85-0P 943007-86-1P
943007-87-2P 943007-88-3P 943007-89-4P 943007-90-7P 943007-91-8P
943007-92-9P 943007-93-0P 943007-94-1P 943007-95-2P 943007-96-3P
943007-97-4P 943007-98-5P 943007-99-6P 943008-00-2P 943008-01-3P
943008-02-4P 943008-03-5P 943008-04-6P 943008-05-7P 943008-06-8P
943008-07-9P 943008-08-0P 943008-09-1P 943008-10-4P 943008-11-5P
943008-12-6P 943008-13-7P 943008-14-8P 943008-15-9P 943008-16-0P
943008-17-1P 943008-18-2P 943008-19-3P 943008-20-6P 943008-21-7P
943008-23-9P 943008-24-0P 943008-25-1P 943008-26-2P 943008-27-3P
943008-28-4P 943008-29-5P 943008-30-8P 943008-31-9P 943008-32-0P
943008-33-1P 943008-34-2P 943008-35-3P 943008-36-4P 943008-37-5P
943008-38-6P 943008-40-0P 943008-41-1P 943008-42-2P 943008-43-3P
943008-44-4P 943008-46-6P 943008-47-7P 943008-49-9P 943008-51-3P
943008-52-4P 943008-55-7P 943008-56-8P 943008-59-1P 943008-60-4P
943008-62-6P 943008-63-7P 943008-66-0P 943008-67-1P 943008-68-2P
943008-69-3P 943008-70-6P 943008-71-7P 943008-72-8P 943008-73-9P
943008-76-2P 943008-77-3P 943008-78-4P 943008-79-5P 943008-80-8P
943008-81-9P 943008-84-2P 943008-85-3P 943008-86-4P 943008-90-0P
943008-92-2P 943008-93-3P 943008-94-4P 943008-95-5P 943008-96-6P
943008-97-7P 943008-98-8P 943008-99-9P 943009-00-5P 943009-01-6P
943009-02-7P 943009-03-8P 943009-05-0P 943009-06-1P 943009-10-7P
943009-11-8P 943009-12-9P 943009-13-0P 943009-14-1P 943009-15-2P
943009-16-3P 943009-17-4P 943009-18-5P 943009-19-6P 943009-20-9P
943009-21-0P 943009-22-1P 943009-23-2P 943009-24-3P 943009-25-4P
943009-26-5P 943009-27-6P 943009-28-7P 943009-30-1P 943009-31-2P
943009-32-3P 943009-33-4P 943009-39-0P 943009-40-3P 943009-41-4P
943009-42-5P 943009-48-1P 943009-50-5P 943009-51-6P 943009-52-7P
943009-53-8P 943009-54-9P 943009-55-0P 943009-56-1P 943009-57-2P
943009-58-3P 943009-59-4P 943009-60-7P 943010-61-5P 943010-63-7P
943010-72-8P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

(Uses)
(preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents)

IT 943009-85-6P 943010-01-3P 943010-83-1P
RL: PEP (Physical, engineering or chemical process); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)
(preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents)

IT 943009-93-6P 943010-05-7P 943010-06-8P
RL: PUR (Purification or recovery); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents)

IT 943010-85-3P 943011-01-6P
RL: PUR (Purification or recovery); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents)

IT 57-56-7, Semicarbazide 75-04-7, Ethylamine, reactions 75-36-5, Acetyl chloride 75-97-8, Pinacolone 79-22-1, Methyl chloroformate 79-44-7, Dimethylcarbamoyl chloride 83-12-5, 2-Phenyl-1,3-indanedione 94-02-0, Ethyl benzoylacetate 95-54-5, 1,2-Phenylenediamine, reactions 96-50-4, 2-Aminothiazole 98-80-6, Phenylboronic acid 98-86-2, Acetophenone, reactions 100-52-7, Benzaldehyde, reactions 103-71-9, Phenyl isocyanate, reactions 110-89-4, Piperidine, reactions 110-91-8, Morpholine, reactions 123-11-5, 4-Methoxybenzaldehyde, reactions 124-40-3, Dimethylamine, reactions 124-63-0, Methanesulfonyl chloride 136-95-8, 2-Aminobenzothiazole 137-07-5, 2-Aminothiophenol 140-29-4, Phenylacetonitrile 288-32-4, Imidazole, reactions 350-03-8, 3-Acetylpyridine 422-59-3, Pentafluoropropionyl chloride 452-58-4, 2,3-Diaminopyridine 504-29-0, 2-Aminopyridine 527-72-0, 2-Thiophenecarboxylic acid 536-74-3, Phenylacetylene 586-75-4, 4-Bromobenzoyl chloride 591-31-1, 3-Methoxybenzaldehyde 616-38-6, Dimethyl carbonate 624-83-9, Methyl isocyanate 703-55-9, 1-Naphthylmagnesium bromide 823-96-1 873-32-5, 2-Chlorobenzonitrile 1066-54-2, Trimethylsilylacetylene 1067-24-9, (Dimethylamino)tributyltin 1067-74-9, Methyl diethylphosphonoacetate 1122-62-9, 2-Acetylpyridine 1122-91-4, 4-Bromobenzaldehyde 1450-93-7, 2-Aminoimidazole hemisulfate 1576-35-8, p-Toluenesulfonyl hydrazide 1589-82-8, Benzylmagnesium bromide 1603-91-4, 2-Amino-4-methylthiazole 1692-15-5, 4-Pyridineboronic acid 1730-25-2, Allylmagnesium bromide 1918-77-0, 2-Thiopheneacetic acid 2289-75-0, 2-Amino-4,5-dimethylthiazole 2393-23-9, 4-Methoxybenzylamine 2605-67-6, Methyl (triphenylphosphoranylidene)acetate 2746-25-0, 4-Methoxybenzyl bromide 2881-83-6, Ethyl 4-methoxybenzoylacetate 3315-91-1, 4-Biphenylylmagnesium bromide 3433-80-5, 2-Bromobenzyl bromide 3724-55-8, Methyl 3-butenoate 4005-51-0, 2-Amino-1,3,4-thiadiazole 4687-37-0, Ethyl 3,4-dimethoxybenzoylacetate 5292-43-3, tert-Butyl bromoacetate 5713-61-1, 2-Thienylmagnesium bromide 6783-05-7, trans-2-Phenylvinylboronic acid 7305-71-7, 2-Amino-5-methylthiazole 7547-97-9, trans-1-Propenylboronic acid 7598-61-0, Diethyl 2,2-diethoxyethylphosphonate 13139-86-1, 4-Methoxyphenylmagnesium bromide 13623-25-1, 6-Methoxy-1-indanone 14527-42-5, Ethyl 2-thiazolecarboxylate 14542-93-9, 1,1,3,3-Tetramethylbutyl isocyanide

14548-39-1, 6-Bromo-1-indanone 16618-72-7, 3-Phenyl-1-indanone 18294-87-6, 1-Cyclohexenylacetic acid 21473-01-8, 2-Naphthylmagnesium bromide 25177-85-9 26466-19-3, 3-Methyl-3-phenyl-1-indanone 27784-76-5, tert-Butyl diethylphosphonoacetate 27834-99-7, Ethyl 3-methoxybenzoylacetate 28987-79-3, 3-Tolylmagnesium bromide 29427-69-8 31775-67-4, trans-2-Aminocyclopentanol hydrochloride 34225-81-5, 3-Methyl-1H-indene-2-carboxylic acid 36282-40-3, 3-Methoxyphenylmagnesium bromide 38205-60-6, 5-Acetyl-2,4-dimethylthiazole 38330-80-2, Potassium methyl malonate 40400-13-3, 2-Iodobenzyl bromide 54696-05-8, 4-Benzyloxyacetophenone 63131-30-6, Ethyl 4-iodobenzoylacetate 64099-82-7, Tributyl(1-propynyl)tin 72824-04-5 79265-30-8, 2-Trimethylsilylthiazole 91350-53-7 95010-17-6 97674-02-7, Tributyl(1-ethoxyvinyl)tin 146794-03-8 172035-86-8, 3-Thienylmagnesium iodide 269410-08-4 405520-68-5 650626-11-2 761446-44-0 861387-14-6 862254-38-4 862254-44-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents)

IT 4254-32-4P 5440-87-9P 7443-02-9P 14190-59-1P, 2-Thiazolecarboxylic acid 14381-42-1P, 1-Indanecarboxylic acid 16440-72-5P 16440-76-9P 22955-78-8P 52957-74-1P 53723-52-7P 93875-76-4P 118215-71-7P 121926-22-5P 121926-30-5P 125868-03-3P 125868-04-4P 126629-81-0P 139592-69-1P 145068-23-1P 154012-99-4P 339116-12-0P 591235-28-8P 943009-61-8P 943009-62-9P 943009-63-0P 943009-64-1P 943009-65-2P 943009-66-3P 943009-67-4P 943009-68-5P 943009-69-6P 943009-71-0P 943009-73-2P 943009-74-3P 943009-75-4P 943009-76-5P 943009-77-6P 943009-78-7P 943009-79-8P 943009-80-1P 943009-81-2P 943009-82-3P 943009-83-4P 943009-84-5P 943009-86-7P 943009-87-8P 943009-88-9P 943009-89-0P 943009-90-3P 943009-91-4P 943009-92-5P 943009-95-8P 943009-96-9P 943009-97-0P 943009-98-1P 943009-99-2P 943010-00-2P 943010-02-4P 943010-03-5P 943010-04-6P 943010-07-9P 943010-08-0P 943010-09-1P 943010-10-4P 943010-11-5P 943010-12-6P 943010-15-9P 943010-17-1P 943010-18-2P 943010-19-3P 943010-20-6P 943010-21-7P 943010-22-8P 943010-23-9P 943010-24-0P 943010-25-1P 943010-26-2P 943010-27-3P 943010-28-4P 943010-29-5P 943010-30-8P 943010-31-9P 943010-32-0P 943010-33-1P 943010-34-2P 943010-35-3P 943010-36-4P 943010-37-5P 943010-38-6P 943010-39-7P 943010-40-0P 943010-41-1P 943010-42-2P 943010-44-4P 943010-45-5P 943010-46-6P 943010-47-7P 943010-48-8P 943010-49-9P 943010-50-2P 943010-51-3P 943010-52-4P 943010-53-5P 943010-54-6P 943010-55-7P 943010-57-9P 943010-58-0P 943010-62-6P 943010-64-8P 943010-65-9P 943010-66-0P 943010-67-1P 943010-68-2P 943010-69-3P 943010-70-6P 943010-71-7P 943010-73-9P 943010-74-0P 943010-75-1P 943010-76-2P 943010-77-3P 943010-78-4P 943010-79-5P 943010-80-8P 943010-81-9P 943010-82-0P 943010-87-5P 943010-88-6P 943010-90-0P 943010-91-1P 943010-92-2P 943010-94-4P 943010-95-5P 943010-97-7P 943010-98-8P 943010-99-9P 943011-00-5P 943011-02-7P 943011-03-8P 943011-04-9P 943011-05-0P 943011-06-1P 943011-11-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents)

IT 9004-10-8, Insulin, biological studies
RL: ADV (Adverse effect, including toxicity); BSU (Biological study, unclassified); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(preparation of indanes as potential modulators of glucocorticoid receptor,

AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents and their use in concert with other agents)

IT 51-61-6, Dopamine, biological studies
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents and their use in concert with other agents)

IT 152755-31-2, LY295427
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents and their use in concert with other agents)

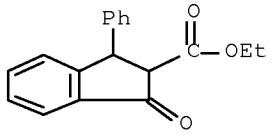
IT 39246-30-5P
RL: BYP (Byproduct); PREP (Preparation)
(regioisomeric byproduct generated in the preparation of an indanecarboxamide as a potential modulator of glucocorticoid receptor, AP-1, or NF-κB activity for use as a antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agent)

IT 943010-56-8P 943010-84-2P 943010-89-7P 943010-93-3P 943010-96-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(undesired diastereomer generated in the preparation of an indanecarboxamide as a potential modulator of glucocorticoid receptor, AP-1, or NF-κB activity for use as a antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agent)

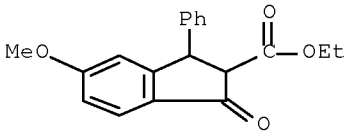
IT 943009-94-7P 943010-86-4P 943011-09-4P
RL: PUR (Purification or recovery); PREP (Preparation)
(undesired enantiomer generated in the preparation of an indanecarboxamide as a potential modulator of glucocorticoid receptor, AP-1, or NF-κB activity for use as a antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agent)

IT 93875-76-4P 154012-99-4P 943009-88-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of indanes as potential modulators of glucocorticoid receptor, AP-1, or NF-κB activity for use as antiobesity, antidiabetic, antiinflammatory, or immunomodulatory agents)

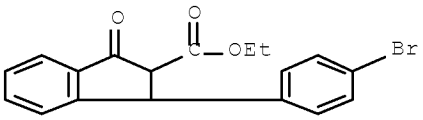
RN 93875-76-4 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 2,3-dihydro-1-oxo-3-phenyl-, ethyl ester (CA INDEX NAME)



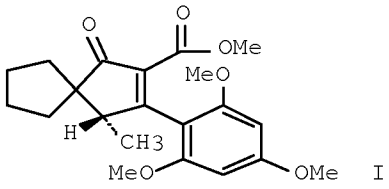
RN 154012-99-4 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 2,3-dihydro-5-methoxy-1-oxo-3-phenyl-, ethyl ester (CA INDEX NAME)



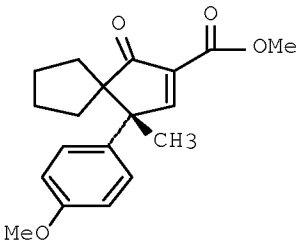
RN 943009-88-9 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-(4-bromophenyl)-2,3-dihydro-3-oxo-, ethyl ester (CA INDEX NAME)



L108 ANSWER 3 OF 21 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2007:626864 ZCAPLUS Full-text
DOCUMENT NUMBER: 147:234758
TITLE: Development of a Nazarov Cyclization/Wagner-Meerwein Rearrangement Sequence for the Stereoselective Synthesis of Spirocycles
AUTHOR(S): Huang, Jie; Frontier, Alison J.
CORPORATE SOURCE: Department of Chemistry, University of Rochester, Rochester, NY, 14627, USA
SOURCE: Journal of the American Chemical Society (2007), 129(26), 8060-8061
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 147:234758
GI



I



II

AB A stereoselective Nazarov cyclization/Wagner-Meerwein rearrangement sequence for the synthesis of spirocyclic compds., e.g. I and II, was developed. While a range of different substrate types engaged in the cyclization/rearrangement sequence, it was found that different substrates underwent different reaction pathways. Depending on the substitution pattern of the substrate, the sequence was terminated by either a hydride shift or the shift of a vinyl or aryl group. It was also possible to install adjacent quaternary stereocenters using this protocol. The efficiency of the Wagner-Meerwein rearrangement was found to be dependent upon both the type and the amount of promoter used to generate the intermediate oxyallyl cation.

CC 24-4 (Alicyclic Compounds)

IT 638186-79-5P

RL: SPN (Synthetic preparation); PREP (Preparation)
(stereoselective synthesis of spirocycles via copper-promoted stereoselective Nazarov cyclization of alkylidene β-ketoesters)

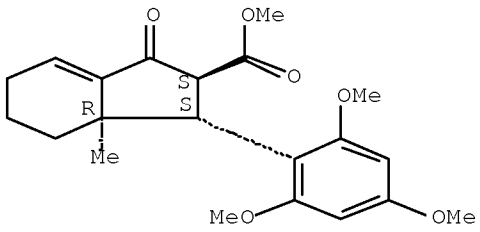
IT 638186-79-5P

RL: SPN (Synthetic preparation); PREP (Preparation)
(stereoselective synthesis of spirocycles via copper-promoted stereoselective Nazarov cyclization of alkylidene β-ketoesters)

RN 638186-79-5 ZCAPLUS

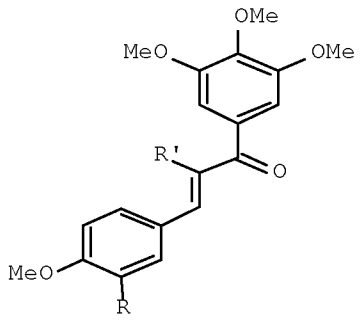
CN 1H-Indene-2-carboxylic acid, 2,3,3a,4,5,6-hexahydro-3a-methyl-1-oxo-3-(2,4,6-trimethoxyphenyl)-, methyl ester, (2R,3R,3aS)-rel- (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L108 ANSWER 4 OF 21 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2007:375477 ZCAPLUS Full-text
DOCUMENT NUMBER: 147:45161
TITLE: The concise synthesis of chalcone, indanone and indenone analogues of combretastatin A4
AUTHOR(S): Kerr, Daniel J.; Hamel, Ernest; Jung, M. Katherine; Flynn, Bernard L.
CORPORATE SOURCE: Department of Medicinal Chemistry, Faculty of Pharmacy, Monash University, Parkville, 3052, Australia
SOURCE: Bioorganic & Medicinal Chemistry (2007), 15(9), 3290-3298
CODEN: BMECEP; ISSN: 0968-0896
PUBLISHER: Elsevier Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

AB A series of aryl- and aroyl-substituted chalcone analogs of the tubulin binding agent combretastatin A4 (1) were prepared, using a recently introduced one-pot palladium-mediated hydrostannylation-coupling reaction sequence. These chalcones were converted to indanones by Nazarov cyclization, followed by oxidation to give the corresponding indenones. Indenones were also prepared using a palladium-mediated formal [3+2]-cycloaddn. process between ortho-halobenzaldehydes and diarylpropynones. All compds. were assessed as inhibitors of tubulin polymerization, but only (I) had activity similar to that of 1. However, I did not exhibit antiproliferative activity against the MCF-7 cell line.

CC 1-3 (Pharmacology)
Section cross-reference(s): 26

ST combretastatin chalcone indanone indenone analog prepn antitumor breast cancer

IT Structure-activity relationship
(antitumor; concise synthesis of chalcone, indanone and indenone analogs of combretastatin A4)

IT Mammary gland, neoplasm
(carcinoma; concise synthesis of chalcone, indanone and indenone analogs of combretastatin A4)

IT Antitumor agents
Human

(concise synthesis of chalcone, indanone and indenone analogs of combretastatin A4)

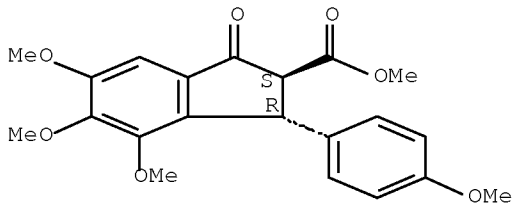
IT Carcinoma
(mammary; concise synthesis of chalcone, indanone and indenone analogs of combretastatin A4)

IT 445483-15-8P 445483-16-9P 446043-31-8P 608533-31-9P 608533-32-0P 608533-33-1P 608533-50-2P 608533-51-3P 939824-63-2P 939824-64-3P 939824-65-4P 939824-66-5P 939824-67-6P 939824-69-8P 939824-71-2P 939824-73-4P 939824-74-5P 939824-75-6P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(concise synthesis of chalcone, indanone and indenone analogs of combretastatin A4)

IT 939824-65-4P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(concise synthesis of chalcone, indanone and indenone analogs of combretastatin A4)

RN 939824-65-4 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 2,3-dihydro-4,5,6-trimethoxy-3-(4-methoxyphenyl)-1-oxo-, methyl ester, (2R,3S)-rel- (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L108 ANSWER 5 OF 21 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2007:194847 ZCAPLUS Full-text
DOCUMENT NUMBER: 146:401667
TITLE: Enantioselective synthesis of 3-arylindan-1-ones via intramolecular C-H insertion reactions of α-diazo-β-ketoesters catalyzed by chiral dirhodium(II) carboxylates
AUTHOR(S): Natori, Yoshihiro; Anada, Masahiro; Nakamura, Seiichi; Nambu, Hisanori; Hashimoto, Shunichi
CORPORATE SOURCE: Faculty of Pharmaceutical Sciences, Hokkaido University, Sapporo, 060-0812, Japan
SOURCE: Heterocycles (2006), 70, 635-646
CODEN: HTCYAM; ISSN: 0385-5414
PUBLISHER: Japan Institute of Heterocyclic Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 146:401667
AB A new, catalytic enantioselective route to 3-arylindan-1-ones (e.g. (S)-3-(3,4-methylenedioxyphenyl)indan-1-one), versatile intermediates for the

synthesis of a number of bioactive and pharmaceutically interesting mols., was developed by exploiting the chiral dirhodium(II) complex-catalyzed intramol. C-H insertion reaction of α-diazo-β- ketoesters (e.g. Me 3-(2-piperonylphenyl)-2-diazo-3-oxopropanoate) as a key step. Dirhodium(II) tetrakis[N-phthaloyl-(S)-tert-leucinate], Rh2(S-PTTL)4, proved to be the catalyst of choice for this process, providing enantioselectivities of up to 72% ee.

CC 25-23 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
Section cross-reference(s): 67

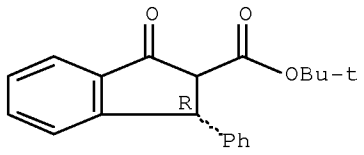
IT 933987-27-0P, tert-Butyl (3R)-3-phenylindan-1-one-2-carboxylate
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(dealkoxycarbonylation; enantioselective synthesis of 3-arylindan-1-ones via intramol. C-H insertion reactions of α-diazo-β-ketoesters catalyzed by chiral dirhodium(II) carboxylates)

IT 933987-21-4P, Methyl (3R)-1-oxo-3-phenylindan-2-carboxylate
933987-23-6P, Methyl (S)-3-(3,4-methylenedioxyphenyl)-1-oxoindane-2-carboxylate
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(demethoxycarbonylation; enantioselective synthesis of 3-arylindan-1-ones via intramol. C-H insertion reactions of α-diazo-β-ketoesters catalyzed by chiral dirhodium(II) carboxylates)

IT 933987-27-0P, tert-Butyl (3R)-3-phenylindan-1-one-2-carboxylate
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(dealkoxycarbonylation; enantioselective synthesis of 3-arylindan-1-ones via intramol. C-H insertion reactions of α-diazo-β-ketoesters catalyzed by chiral dirhodium(II) carboxylates)

RN 933987-27-0 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 2,3-dihydro-1-oxo-3-phenyl-, 1,1-dimethylethyl ester, (3R)- (CA INDEX NAME)

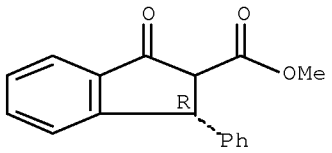
Absolute stereochemistry.



IT 933987-21-4P, Methyl (3R)-1-oxo-3-phenylindan-2-carboxylate
933987-23-6P, Methyl (S)-3-(3,4-methylenedioxyphenyl)-1-oxoindane-2-carboxylate
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(demethoxycarbonylation; enantioselective synthesis of 3-arylindan-1-ones via intramol. C-H insertion reactions of α-diazo-β-ketoesters catalyzed by chiral dirhodium(II) carboxylates)

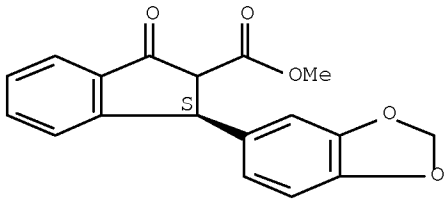
RN 933987-21-4 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 2,3-dihydro-1-oxo-3-phenyl-, methyl ester, (3R)- (CA INDEX NAME)

Absolute stereochemistry.



RN 933987-23-6 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-(1,3-benzodioxol-5-yl)-2,3-dihydro-3-oxo-, methyl ester, (1S)- (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 44 THERE ARE 44 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L108 ANSWER 6 OF 21 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2005:510329 ZCAPLUS Full-text
DOCUMENT NUMBER: 143:172430
TITLE: Preorganization in the Nazarov cyclization: the role of adjacent coordination sites in the highly Lewis acidic catalyst [IrMe(CO)(dppe)(DIB)](BArf4)2
AUTHOR(S): Janka, Mesfin; He, Wei; Frontier, Alison J.; Flaschenriem, Christine; Eisenberg, Richard
CORPORATE SOURCE: Department of Chemistry, University of Rochester, Rochester, NY, 14627, USA
SOURCE: Tetrahedron (2005), 61(26), 6193-6206
CODEN: TETRAB; ISSN: 0040-4020
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 143:172430
AB The dicationic Ir(III) complex [IrMe(CO)(dppe)(DIB)](BAr4 f)2 where dppe=bis(diphenylphosphino)ethane and DIB=o-diiodobenzene possesses adjacent labile sites and is found to be a very active catalyst for the Nazarov cyclization. 31P NMR spectroscopy provides evidence for substrate-catalyst binding by chelation, and this is found to be the resting state of the system during catalysis. The efficiency of the cyclization is attributed to the electrophilicity of the Ir(III) complex and substrate activation via O,O'-chelation which employs two substrate carbonyl groups or one carbonyl and an ether function, and encourages the s-trans/s-trans conformation required for cyclization. When two point binding occurs through an oxygen atom and one of the vinyl groups, the s-trans/s-trans conformation is not achieved, and

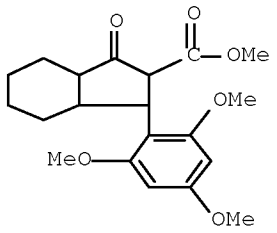
cyclization is not observed In one case, monodentate binding of substrate occurs, and the rate of cyclization is significantly slower than when O,O'-chelation is possible. The viability of O,O'-chelation is shown by the crystal structure determination of a model substrate-catalyst complex.

CC 22-5 (Physical Organic Chemistry)
Section cross-reference(s): 29

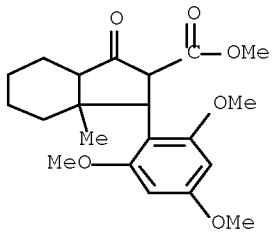
IT 861215-41-0P 879044-33-4P 879048-60-9P 879055-02-4P
879080-18-9P 879080-36-1P 879080-37-2P 879080-38-3P
879080-70-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(role of adjacent coordination sites in the highly Lewis acidic Nazarov cyclization catalyst [IrMe(CO)(dppe)(DIB)](BArf4)2)

IT 879080-18-9P 879080-37-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(role of adjacent coordination sites in the highly Lewis acidic Nazarov cyclization catalyst [IrMe(CO)(dppe)(DIB)](BArf4)2)

RN 879080-18-9 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, octahydro-1-oxo-3-(2,4,6-trimethoxyphenyl)-, methyl ester (CA INDEX NAME)



RN 879080-37-2 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, octahydro-3a-methyl-1-oxo-3-(2,4,6-trimethoxyphenyl)-, methyl ester (CA INDEX NAME)

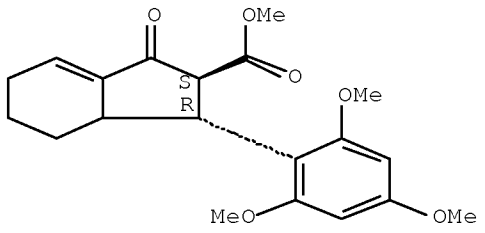


REFERENCE COUNT: 56 THERE ARE 56 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L108 ANSWER 7 OF 21 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2004:603163 ZCAPLUS Full-text
DOCUMENT NUMBER: 142:261224
TITLE: Polarizing the Nazarov cyclization: efficient catalysis under mild conditions. [Erratum to document cited in CA140:059334]

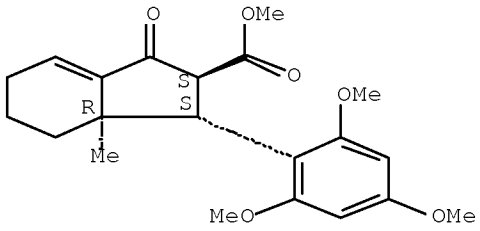
AUTHOR(S): He, Wei; Sun, Xiufeng; Frontier, Alison J.
CORPORATE SOURCE: Department of Chemistry, University of Rochester, Rochester, NY, 14627, USA
SOURCE: Journal of the American Chemical Society (2004), 126(33), 10493
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB On page 14278, Table 2, compound 12a was represented by the wrong drawing (a different epimer). The corrected drawing represents the x-ray crystal structure data reported in the Supporting Information.
CC 24-4 (Alicyclic Compounds)
Section cross-reference(s): 27
IT 638186-64-8P 638186-65-9P 638186-66-0P 638186-67-1P 638186-68-2P
638186-69-3P 638186-75-1P 638186-76-2P 638186-78-4P
638186-79-5P 638186-80-8P 638186-81-9P 638186-83-1P
638186-85-3P 638186-87-5P 638186-89-7P 638186-91-1P
638186-92-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(regio- and stereoselective preparation of polysubstituted and fused cyclopentenones via copper-catalyzed polarized Nazarov cyclization of functionalized divinyl ketones (Erratum))
IT 638186-75-1P 638186-79-5P 638186-91-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(regio- and stereoselective preparation of polysubstituted and fused cyclopentenones via copper-catalyzed polarized Nazarov cyclization of functionalized divinyl ketones (Erratum))
RN 638186-75-1 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 2,3,3a,4,5,6-hexahydro-1-oxo-3-(2,4,6-trimethoxyphenyl)-, methyl ester, (2R,3S)-rel- (CA INDEX NAME)

Relative stereochemistry.



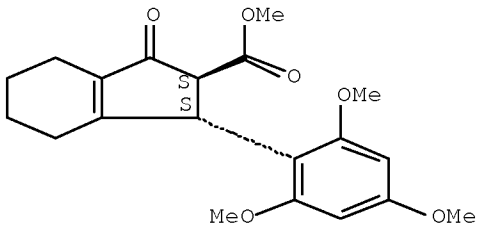
RN 638186-79-5 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 2,3,3a,4,5,6-hexahydro-3a-methyl-1-oxo-3-(2,4,6-trimethoxyphenyl)-, methyl ester, (2R,3R,3aS)-rel- (CA INDEX NAME)

Relative stereochemistry.



RN 638186-91-1 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 2,3,4,5,6,7-hexahydro-1-oxo-3-(2,4,6-trimethoxyphenyl)-, methyl ester, (2R,3R)-rel- (CA INDEX NAME)

Relative stereochemistry.



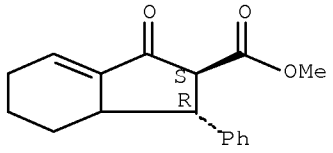
L108 ANSWER 8 OF 21 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2004:400197 ZCAPLUS Full-text
DOCUMENT NUMBER: 141:106095
TITLE: Efficient Catalysis of Nazarov Cyclization Using a Cationic Iridium Complex Possessing Adjacent Labile Coordination Sites
AUTHOR(S): Janka, Mesfin; He, Wei; Frontier, Alison J.; Eisenberg, Richard
CORPORATE SOURCE: Department of Chemistry, University of Rochester, Rochester, NY, 14627, USA
SOURCE: Journal of the American Chemical Society (2004), 126(22), 6864-6865
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 141:106095
AB The dicationic Ir(III) complex [IrMe(CO)(dppe)(DIB)](BARF)2 having adjacent labile sites has been found to be a very effective catalyst for promoting the Nazarov cyclization of aryl vinyl and divinyl ketones. Spectroscopic evidence for a substrate-catalyst complex before cyclization is presented. The efficiency of the cyclization is attributed to the electrophilicity of the Ir(III) complex and substrate activation via chelation.
CC 22-5 (Physical Organic Chemistry)
Section cross-reference(s): 29, 67
IT 638186-64-8P 638186-65-9P 638186-66-0P 638186-67-1P 638186-68-2P 638186-69-3P 638186-78-4P 638186-81-9P 716323-94-3P 716323-95-4P

RL: SPN (Synthetic preparation); PREP (Preparation)
(efficient catalysis of Nazarov cyclization using a cationic iridium complex possessing adjacent labile coordination sites)

IT 716323-94-3P 716323-95-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(efficient catalysis of Nazarov cyclization using a cationic iridium complex possessing adjacent labile coordination sites)

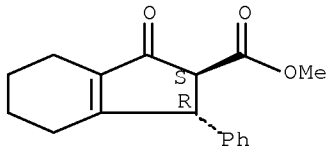
RN 716323-94-3 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 2,3,3a,4,5,6-hexahydro-1-oxo-3-phenyl-, methyl ester, (2R,3S)-rel- (CA INDEX NAME)

Relative stereochemistry.



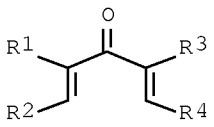
RN 716323-95-4 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 2,3,4,5,6,7-hexahydro-1-oxo-3-phenyl-, methyl ester, (2R,3S)-rel- (CA INDEX NAME)

Relative stereochemistry.

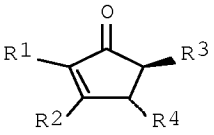


REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L108 ANSWER 9 OF 21 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2003:847382 ZCAPLUS Full-text
DOCUMENT NUMBER: 140:59334
TITLE: Polarizing the Nazarov Cyclization: Efficient Catalysis under Mild Conditions
AUTHOR(S): He, Wei; Sun, Xiufeng; Frontier, Alison J.
CORPORATE SOURCE: Department of Chemistry, University of Rochester, Rochester, NY, 14627, USA
SOURCE: Journal of the American Chemical Society (2003), 125(47), 14278-14279
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 140:59334
GI



I



II

AB Substituted divinyl ketones were studied in the Nazarov cyclization. Divinyl ketones I [R1, R2 = H, Me; R1R2 = (CH2)5, O(CH2)3, etc.; R3 = H, MeO2C; R4 = Ph, 2,4,6-(MeO)3C6H2, 2-furyl, cyclohexyl, etc.] underwent efficient Nazarov cyclization with catalytic copper triflate (2 mol %) to give the corresponding cyclopentenones II as single regio- and stereoisomers. The efficiency of the cyclizations correlated with the ability of the substituents to favorably polarize the π-system of the cationic intermediate.

CC 24-4 (Alicyclic Compounds)
Section cross-reference(s): 27

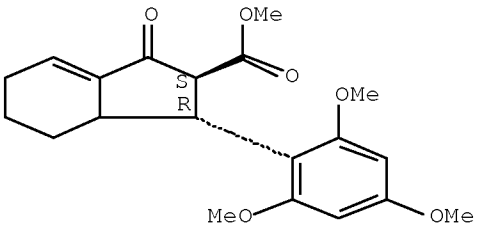
IT 638186-64-8P 638186-65-9P 638186-66-0P 638186-67-1P 638186-68-2P
638186-69-3P 638186-75-1P 638186-76-2P 638186-78-4P
638186-79-5P 638186-80-8P 638186-81-9P 638186-83-1P
638186-85-3P 638186-87-5P 638186-89-7P 638186-91-1P
638186-92-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(regio- and stereoselective preparation of polysubstituted and fused cyclopentenones via copper-catalyzed polarized Nazarov cyclization of functionalized divinyl ketones)

IT 638186-75-1P 638186-79-5P 638186-91-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(regio- and stereoselective preparation of polysubstituted and fused cyclopentenones via copper-catalyzed polarized Nazarov cyclization of functionalized divinyl ketones)

RN 638186-75-1 ZCAPLUS

CN 1H-Indene-2-carboxylic acid, 2,3,3a,4,5,6-hexahydro-1-oxo-3-(2,4,6-trimethoxyphenyl)-, methyl ester, (2R,3S)-rel- (CA INDEX NAME)

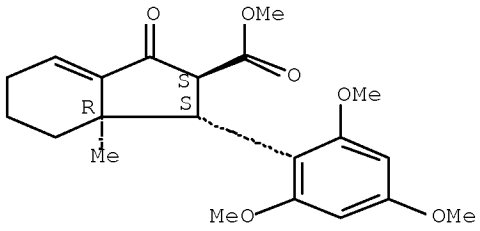
Relative stereochemistry.



RN 638186-79-5 ZCAPLUS

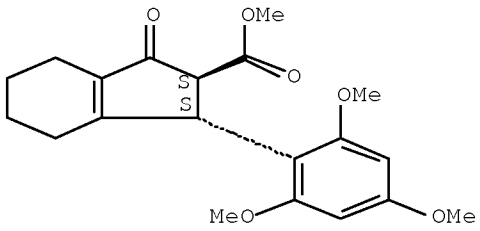
CN 1H-Indene-2-carboxylic acid, 2,3,3a,4,5,6-hexahydro-3a-methyl-1-oxo-3-(2,4,6-trimethoxyphenyl)-, methyl ester, (2R,3R,3aS)-rel- (CA INDEX NAME)

Relative stereochemistry.



RN 638186-91-1 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 2,3,4,5,6,7-hexahydro-1-oxo-3-(2,4,6-trimethoxyphenyl)-, methyl ester, (2R,3R)-rel- (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L108 ANSWER 10 OF 21 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2003:415838 ZCAPLUS Full-text
DOCUMENT NUMBER: 139:292182
TITLE: A convenient two step protocol for the synthesis of cyclopentenones and indanones, including an asymmetric variant
AUTHOR(S): Kerr, Daniel J.; Metje, Christiane; Flynn, Bernard L.
CORPORATE SOURCE: Department of Chemistry, The Faculties, Australian National University, Canberra, 0200, Australia
SOURCE: Chemical Communications (Cambridge, United Kingdom) (2003), (12), 1380-1381
CODEN: CHCOFS; ISSN: 1359-7345
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 139:292182
AB A one-pot palladium mediated hydrostannylation/cross-coupling protocol is used to give direct access to cross-conjugated dienones that can be utilized in Nazarov cyclizations to afford highly substituted cyclopentenones and indanones, including an asym. variant. Palladium-mediated hydrostannylation of (4S)-3-(1-oxo-3-phenyl-2-propynyl)- 4-phenyl-2-oxazolidinone, followed by addition of (2E)-2-methyl-2-butenoyl chloride gave (4S)-4-phenyl-3-[(2Z,4E)-2-(phenylmethylene)-4-methyl-1,3- dioxo-4-hexenyl]-2-oxazolidione. Subsequent Nazarov cyclization of the latter gave (4S)-3-[(1S,2S)-(3,4-dimethyl-5-oxo-2-phenyl-3-cyclopenten-1- yl)carbonyl]-4-phenyl-2-oxazolidinone. This product

isomerized to (4S)-3-[(1R,2S)-(3,4-dimethyl-5-oxo-2-phenyl-3-cyclopenten-1-yl)carbonyl]- 4-phenyl-2-oxazolidinone.

CC 28-6 (Heterocyclic Compounds (More Than One Hetero Atom))

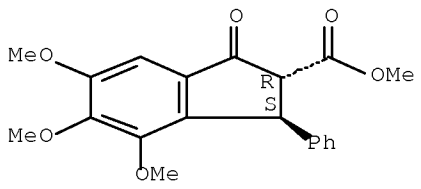
IT 42443-26-5P 446043-40-9P 608533-23-9P 608533-24-0P 608533-25-1P
608533-27-3P 608533-31-9P 608533-32-0P 608533-33-1P 608533-34-2P
608533-35-3P 608533-36-4P 608533-37-5P 608533-38-6P
608533-39-7P 608533-40-0P 608533-41-1P 608533-42-2P 608533-43-3P
608533-44-4P 608533-45-5P 608533-46-6P 608533-47-7P 608533-48-8P
608533-49-9P 608533-50-2P 608533-51-3P 608533-52-4P 608533-53-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of cyclopentenones and indanones via palladium-mediated hydrostannylation/cross-coupling)

IT 608533-38-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of cyclopentenones and indanones via palladium-mediated hydrostannylation/cross-coupling)

RN 608533-38-6 ZCAPLUS

CN 1H-Indene-2-carboxylic acid, 2,3-dihydro-4,5,6-trimethoxy-1-oxo-3-phenyl-, methyl ester, (2R,3S)-rel- (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

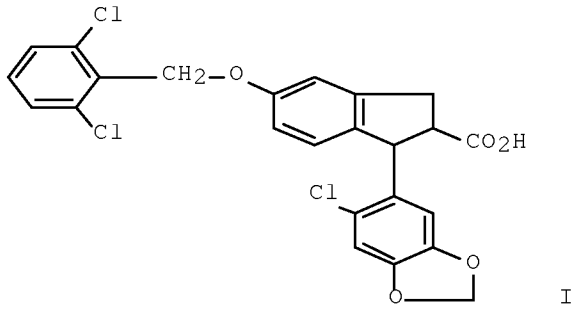
L108 ANSWER 11 OF 21 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2002:31260 ZCAPLUS Full-text
DOCUMENT NUMBER: 136:102198
TITLE: Indan derivatives as fatty acid synthase inhibitors
INVENTOR(S): Xiang, Jia-Ning; Christensen, Siegfried B., IV; Mercer, Daniel J.
PATENT ASSIGNEE(S): Smithkline Beecham Corporation, USA
SOURCE: PCT Int. Appl., 22 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002002119	A1	20020110	WO 2001-US20926	20010629

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

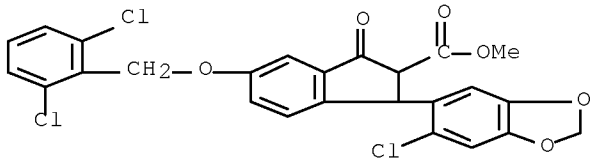
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,

DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
PRIORITY APPLN. INFO.: US 2000-214889P P 20000629
OTHER SOURCE(S): MARPAT 136:102198
GI



I

AB This invention relates to the use of compds. as inhibitors of the fatty acid synthase FabH. E.g., I was prepared and biol. assays were described.
IC ICM A61K031-50
ICS A61K031-18; C07D231-02; C07C321-00; C07C315-00
CC 25-23 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
Section cross-reference(s): 1, 28, 63
IT 202144-69-2P 387844-34-0P 387844-35-1P 387844-36-2P
387844-37-3P 387844-38-4P 387844-39-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(indan derivs. as fatty acid synthase inhibitors)
IT 387844-36-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(indan derivs. as fatty acid synthase inhibitors)
RN 387844-36-2 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-(6-chloro-1,3-benzodioxol-5-yl)-5-[(2,6-dichlorophenyl)methoxy]-2,3-dihydro-3-oxo-, methyl ester (CA INDEX NAME)



REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

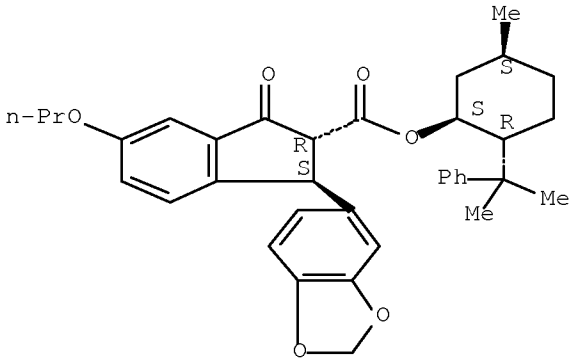
L108 ANSWER 12 OF 21 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1999:646301 ZCAPLUS Full-text

DOCUMENT NUMBER: 131:299386
TITLE: An unprecedented asymmetric Nazarov cyclization for the synthesis of nonracemic indanes as endothelin receptor antagonists
AUTHOR(S): Pridgen, Lendon N.; Huang, Kris; Shilcrat, Susan; Tickner-Eldridge, Ann; DeBrosse, Charles; Haltiwanger, R. Curtis
CORPORATE SOURCE: Synthetic Chemistry Dep., SmithKline Beecham Pharmaceuticals, King of Prussia, PA, 19406, USA
SOURCE: Synlett (1999), (10), 1612-1614
CODEN: SYNLES; ISSN: 0936-5214
PUBLISHER: Georg Thieme Verlag
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 131:299386

AB An asym. synthesis of the novel nonracemic endothelin receptor antagonists SB 209670 and SB 217242 is described which utilizes an unprecedented asym. Nazarov-type ring-closure of alkylidene 1,3-dicarbonyl compds. Excellent 1,5-induction is observed which establishes the required S configuration at C(3) of an indane skeleton.

CC 28-5 (Heterocyclic Compounds (More Than One Hetero Atom))
IT 247057-29-0P 247057-30-3P 247057-31-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of indanes as precursors of SB 209670 and SB 217242 by asym. Nazarov cyclization)
IT 247057-31-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of indanes as precursors of SB 209670 and SB 217242 by asym. Nazarov cyclization)
RN 247057-31-4 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-(1,3-benzodioxol-5-yl)-2,3-dihydro-3-oxo-5-propoxy-, (1R,2S,5R)-5-methyl-2-(1-methyl-1-phenylethyl)cyclohexyl ester, (1R,2S)-rel- (CA INDEX NAME)

Relative stereochemistry.



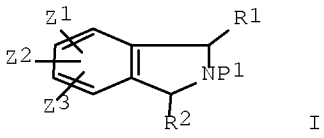
REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L108 ANSWER 13 OF 21 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1999:468065 ZCAPLUS Full-text
DOCUMENT NUMBER: 131:116225
TITLE: Preparation of isoindole derivatives as endothelin

receptor antagonists
INVENTOR(S): Elliott, John Duncan; Franz, Robert Gene; Lago, M. Amparo; Gao, Aiming
PATENT ASSIGNEE(S): Smithkline Beecham Corp., USA
SOURCE: U.S., 9 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5929106	A	19990727	US 1997-958781	19971027
PRIORITY APPLN. INFO.:			US 1997-958781	19971027

OTHER SOURCE(S): MARPAT 131:116225
GI



I

AB Dihydroisoindole compds. of formula [I; R1 = X (CH2)nR8; R2 = H, Ar, C1-4 alkyl; P1 = tetrazolyl, SO2R7R11, (CH2)5CO2R7; Z1, Z2 = H, C1-8 alkyl, C2-8 alkenyl, C2-8 alkynyl, OH, C1-8 alkoxy, C1-8 alkyl-(S)q, (un)substituted NH2, Br, F, iodo, NHCHO, C1-4 alkylcarbonylamino, Ph, CH2Ph, etc.; or Z1 and Z2 together may be O-A-O on contiguous carbons; wherein A = CO, (un)substituted CH2; Z3 = Z1, X-R9-Y; X = (CH2)n, O, (un)substituted NH; wherein Y = Me, X(CH2)nAr; wherein R7 = H, C1-10 alkyl, C2-10 alkenyl, C2-8 alkynyl, (CH2)nAr; R8 = R11, CO2R7, CO2C(R11)2O2CXR7, PO3(R7)2, SO2NR7R11, NR7SO2R11, CONR7SO2R11, SO3R7, SO2R7, cyano, etc.; R9 = (CH2)n, C1-10 alkylene, C2-10 alkenylene, phenylenyl, CO, C1-5 alkyl-X; R11 = H, Ar, C1-8 alkylene, C2-8 alkenylene, C2-8 alkynylene, etc.;Ar = (un)substituted Ph, naphthyl, indolyl, pyridyl, thienyl, oxazolidinyl, oxazolyl, thiazolyl, isothiazolyl, pyrazolyl, triazolyl, tetrazolyl, imidazolyl, imidazolidinyl, thiazolidinyl, isoxazolyl, oxadiazolyl, thiadiazolyl, morpholinyl, piperidinyl, piperazinyl, pyrrolyl, pyrimidyl, etc.; wherein n = 0-6; q = 0-2] are prepared The compds. are applied in the treatment of hypertension and cardiovascular and renal diseases. Thus, Me (1RS,3RS)-3-[(2-hydroxy-4- methoxy)phenyl]-1-(3,4-methylenedioxyphenyl)-5-prop-1-yloxy-(1H,3H- dihydroisoindol-2-yl)acetate in dry DMF was added potassium carbonate under argon, stirred at room temperature for 20 min, then treated with Et bromoacetate, and stirred for 24 h, followed by saponification and acidification, to give the title compound (II). Title compds. inhibited [125 I]ET-1 binding to membranes from rat cerebellum or kidney cortex or CHO cell membranes with IC50 of 0.01 nm to 50 μM and ET-1-induced vascular contraction using rat aorta with dissociation constant of 0.1 nM to 50 nM as competitive antagonists.

IC ICM A61K031-405
ICS C07D209-10
INCL 514414000
CC 28-5 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1

ST isoindole prepn endothelin receptor antagonist; hypertension treatment isoindole; cardiovascular disease treatment isoindole; renal disease treatment isoindole

IT Endothelin receptors
RL: BPR (Biological process); BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study); PROC (Process)
(preparation of isoindole derivs. as endothelin receptor antagonists for treatment of hypertension and cardiovascular and renal diseases)

IT 232602-97-0P 232602-98-1P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of isoindole derivs. as endothelin receptor antagonists for treatment of hypertension and cardiovascular and renal diseases)

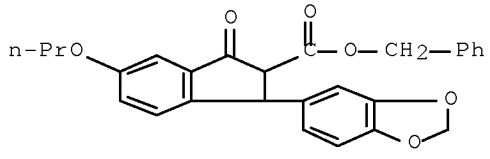
IT 96-35-5, Methyl glycolate 100-51-6, Benzyl alcohol, reactions 100-66-3, Anisole, reactions 120-57-0, 3,4-(Methylenedioxy)benzaldehyde 358-23-6, Triflic anhydride 21615-34-9, o-Methoxybenzoyl chloride 62646-09-7 150356-60-8 205640-56-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of isoindole derivs. as endothelin receptor antagonists for treatment of hypertension and cardiovascular and renal diseases)

IT 4136-21-4P, 2-Hydroxy-4'-methoxyacetophenone 88016-31-3P 174527-87-8P 174527-88-9P 174527-89-0P 174527-90-3P 174527-91-4P 174527-92-5P 174527-98-1P 174527-99-2P 174528-02-0P 205640-51-3P 232602-99-2P 232603-00-8P 232603-01-9P 232603-02-0P 232603-03-1P 232603-04-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of isoindole derivs. as endothelin receptor antagonists for treatment of hypertension and cardiovascular and renal diseases)

IT 232602-99-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of isoindole derivs. as endothelin receptor antagonists for treatment of hypertension and cardiovascular and renal diseases)

RN 232602-99-2 ZCAPLUS

CN 1H-Indene-2-carboxylic acid, 1-(1,3-benzodioxol-5-yl)-2,3-dihydro-3-oxo-5-propoxy-, phenylmethyl ester (CA INDEX NAME)



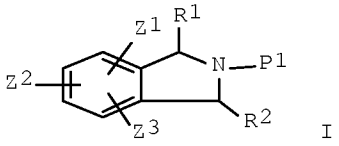
REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L108 ANSWER 14 OF 21 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1998:219350 ZCAPLUS Full-text
DOCUMENT NUMBER: 128:270534

ORIGINAL REFERENCE NO.: 128:53553a,53556a
TITLE: Dihydroisoindole compounds Endothelin receptor antagonists
INVENTOR(S): Elliott, John Duncan; Franz, Robert Gene; Lago, M. Amparo; Gao, Aiming
PATENT ASSIGNEE(S): Smithkline Beecham Corporation, USA
SOURCE: U.S., 9 pp., Cont.-in-part of U.S. Ser. No. 262,801. CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5736564	A	19980407	US 1996-464761	19961212
WO 9535107	A1	19951228	WO 1995-US7193	19950606
W: JP, US				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				

PRIORITY APPLN. INFO.: US 1994-262801 A2 19940620
WO 1995-US7193 W 19950606
OTHER SOURCE(S): MARPAT 128:270534
GI



I

AB Compds. I [R1 = X(CH2)nAr; R2 = H, Ar, C1-4 alkyl; P1 = tetrazole, SO2NR7R11, CONR7SO2R11, (CH2)sR8; R3, R5 = H, halo, R11, OH, etc.; R4 = H, halo, R11, C1-5 alkoxy, etc.; R6 = H, C1-4 alkyl; R7 = H, (un)substituted C1-10 alkyl, C2-10 alkenyl, C2-8 alkynyl, etc.; R8 = H, R11, CO2R7, etc.; R9 = (CH2)n, C1-10 alkylene, C2-10 alkenylene, etc.; R11 = H, C1-8 alkylene, C2-8 alkenylene, etc.; X = (CH2)n, O, NR6; Y = Me, X(CH2)nAr; Ar = naphthyl, indolyl, pyridyl, etc.; Z1, Z2 = H, C1-8 alkyl, C2-8 alkenyl, etc.; Z3 = Z1, XR9Y; n = 0-6; s = 1-6] and pharmaceutical compns. containing I, which are useful for endothelin receptor antagonists, are prepared The IC50's for the compds. range from 0.01 nm to 50 μM. The compds. are useful in the treatment of hypertension, renal failure, and cerebrovascular diseases. Thus, (1RS, 3RS)-3-[(2-carboxymethoxy-4- methoxy)phenyl]-1-(3,4-methylenedioxyphenyl)-5-prop-1-yloxy-(1H,3H-dihydro-isoindol-2-yl)acetic acid trifluoroacetate salt and (1RS,3RS)-3-(4-methoxyphenyl)-1-(3,4-methylenedioxyphenyl)-(1H,3H-dihydroisoindol-2-yl)acetic acid were prepared

IC ICM A61K031-40
ICS C07D209-08
INCL 514414000
CC 27-11 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 1, 63
ST dihydroisoindole endothelin receptor antagonist; hypertension treatment dihydroisoindole; renal failure treatment dihydroisoindole; cerebrovascular disease treatment dihydroisoindole
IT Antihypertensives

(dihydroisoindole compds. and pharmaceutical compns. for endothelin receptor antagonists)

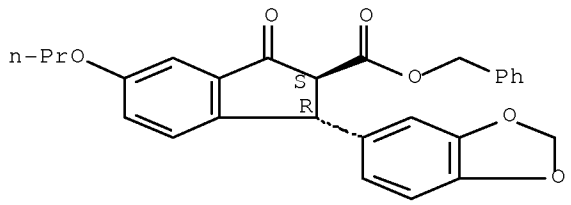
IT 4136-21-4P, 2-Hydroxy-4'-methoxyacetophenone 88016-31-3P 174527-87-8P 174527-88-9P 174527-89-0P 174527-90-3P 174527-91-4P 174527-92-5P 174527-93-6P 174527-94-7P 174527-95-8P 174527-97-0P 174527-98-1P 174527-99-2P 174528-00-8P 174528-01-9P 174528-02-0P 205640-51-3P 205640-52-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(dihydroisoindole compds. and pharmaceutical compns. for endothelin receptor antagonists)

IT 205640-52-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(dihydroisoindole compds. and pharmaceutical compns. for endothelin receptor antagonists)

RN 205640-52-4 ZCAPLUS

CN 1H-Indene-2-carboxylic acid, 1-(1,3-benzodioxol-5-yl)-2,3-dihydro-3-oxo-5-propoxy-, phenylmethyl ester, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L108 ANSWER 15 OF 21 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1996:170769 ZCAPLUS Full-text
DOCUMENT NUMBER: 124:194314
ORIGINAL REFERENCE NO.: 124:35679a,35682a
TITLE: Dihydroisoindole endothelin receptor antagonists, their preparation, pharmaceuticals containing them, and their therapeutic use
INVENTOR(S): Elliott, John Duncan; Franz, Robert Gene; Lago, Maria Amparo; Gao, Aiming
PATENT ASSIGNEE(S): SmithKline Beecham Corp., USA
SOURCE: PCT Int. Appl., 27 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9535107	A1	19951228	WO 1995-US7193	19950606
W: JP, US				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
EP 768878	A1	19970423	EP 1995-921616	19950606

R: BE, CH, DE, FR, GB, IT, LI, NL

JP 10501812	T	19980217	JP 1995-502309		19950606
US 5736564	A	19980407	US 1996-464761		19961212
PRIORITY APPLN. INFO.:			US 1994-262801	A	19940620
			WO 1995-US7193	W	19950606

AB Dihydroisoindole compds. (Markush included) are disclosed as being useful as endothelin receptor antagonists. The compds. may be applied in the treatment of cardiovascular and renal diseases. Preparation of e.g. (1RS, 3RS)-3-(4-methoxyphenyl)-1-(3,4-methylenedioxyphenyl)-(1H, 3H-dihydroisoindol-2-yl)acetic acid is included, as are pharmaceutical formulations. In a radioiodinated endothelin-1 binding protocol, compds. of the invention have IC50 values in the range 0.01 nM to 50 μM.

IC ICM A61K031-40
ICS A61K031-41; C07D209-44; C07D403-04

CC 1-8 (Pharmacology)
Section cross-reference(s): 27

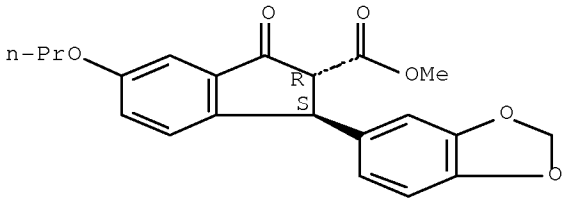
IT Antihypertensives
Cardiovascular agents
Pharmaceutical dosage forms
(dihydroisoindole endothelin receptor antagonists, preparation, pharmaceuticals, and therapeutic use)

IT 4136-21-4P, 2-Hydroxy-4'-methoxyacetophenone 88016-31-3P
150356-61-9P 174527-85-6P 174527-87-8P 174527-88-9P
174527-89-0P 174527-90-3P 174527-91-4P 174527-92-5P 174527-93-6P
174527-94-7P 174527-95-8P 174527-97-0P 174527-98-1P 174527-99-2P
174528-00-8P 174528-01-9P 174528-02-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(dihydroisoindole endothelin receptor antagonists, preparation, pharmaceuticals, and therapeutic use)

IT 150356-61-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(dihydroisoindole endothelin receptor antagonists, preparation, pharmaceuticals, and therapeutic use)

RN 150356-61-9 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-(1,3-benzodioxol-5-yl)-2,3-dihydro-3-oxo-5-propoxy-, methyl ester, (1R,2S)-rel- (CA INDEX NAME)

Relative stereochemistry.



L108 ANSWER 16 OF 21 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1995:908977 ZCAPLUS Full-text
DOCUMENT NUMBER: 124:116823
ORIGINAL REFERENCE NO.: 124:21753a,21756a
TITLE: Selective synthesis of 1-indanones via tandem Knoevenagel condensation-cycloalkylation of

β-dicarbonyl compounds and aldehydes
AUTHOR(S): Sartori, Giovanni; Maggi, Raimondo; Bigi, Franca; Porta, Cecilia; Tao, Xiaochun; Bernardi, Gian Luca; Ianelli, Sandra; Nardelli, Mario
CORPORATE SOURCE: Dip. Chim. Org. Industriale dell'Universita, Parma, I-43100, Italy
SOURCE: Tetrahedron (1995), 51(44), 12179-92
CODEN: TETRAB; ISSN: 0040-4020
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 124:116823

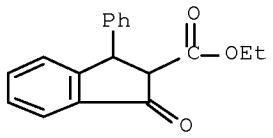
AB Aromatic 1,3-dicarbonyl compds. react with non-enolizable aldehydes in the presence of C2H5MgBr or AlCl3 affording 2-carbethoxy- and 2-acetyl-1-indanones via tandem Knoevenagel condensation-cycloalkylation process.

CC 25-25 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)

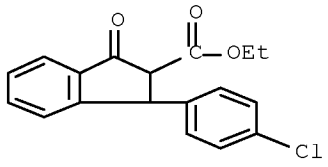
IT 5350-68-5P 6742-25-2P 65805-51-8P 77404-33-2P 93875-76-4P 154012-97-2P 154012-98-3P 154013-00-0P 173031-20-4P 173031-21-5P 173031-22-6P 173031-23-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

IT 93875-76-4P 154012-97-2P 154012-98-3P 173031-22-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

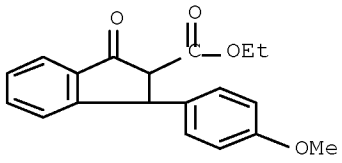
RN 93875-76-4 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 2,3-dihydro-1-oxo-3-phenyl-, ethyl ester (CA INDEX NAME)



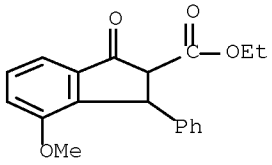
RN 154012-97-2 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 1-(4-chlorophenyl)-2,3-dihydro-3-oxo-, ethyl ester (CA INDEX NAME)



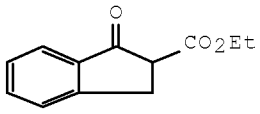
RN 154012-98-3 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 2,3-dihydro-1-(4-methoxyphenyl)-3-oxo-, ethyl ester (CA INDEX NAME)



RN 173031-22-6 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 2,3-dihydro-4-methoxy-1-oxo-3-phenyl-, ethyl ester (CA INDEX NAME)



L108 ANSWER 17 OF 21 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1994:244284 ZCAPLUS Full-text
DOCUMENT NUMBER: 120:244284
ORIGINAL REFERENCE NO.: 120:43281a,43284a
TITLE: Friedel-Crafts coordinated processes: 1-oxoindans from aromatic β-dicarbonyl compounds and aldehydes
AUTHOR(S): Sartori, Giovanni; Bigi, Franca; Maggi, Raimondo; Bernardi, Gian Luca
CORPORATE SOURCE: Dip. Chim. Org. Ind., Univ. Parma, Parma, I-43100, Italy
SOURCE: Tetrahedron Letters (1993), 34(45), 7339-42
CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 120:244284
GI



I

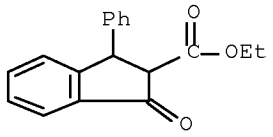
AB Variously substituted 1-oxoindans, e.g., I, were synthesized by highly selective bis-alkylation of aromatic β-dicarbonyl compds., e.g., BzCO2Et, with nonenolizable aldehydes, e.g., HCHO.
CC 25-23 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
IT 5350-68-5P 6742-25-2P 16425-82-4P 77404-33-2P 93875-76-4P

144067-28-7P 154012-97-2P 154012-98-3P
154012-99-4P 154013-00-0P 154013-01-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

IT 93875-76-4P 154012-97-2P 154012-98-3P
154012-99-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

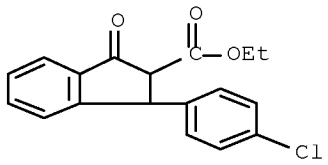
RN 93875-76-4 ZCAPLUS

CN 1H-Indene-2-carboxylic acid, 2,3-dihydro-1-oxo-3-phenyl-, ethyl ester (CA INDEX NAME)



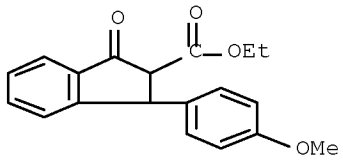
RN 154012-97-2 ZCAPLUS

CN 1H-Indene-2-carboxylic acid, 1-(4-chlorophenyl)-2,3-dihydro-3-oxo-, ethyl ester (CA INDEX NAME)



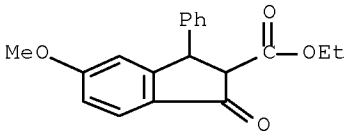
RN 154012-98-3 ZCAPLUS

CN 1H-Indene-2-carboxylic acid, 2,3-dihydro-1-(4-methoxyphenyl)-3-oxo-, ethyl ester (CA INDEX NAME)

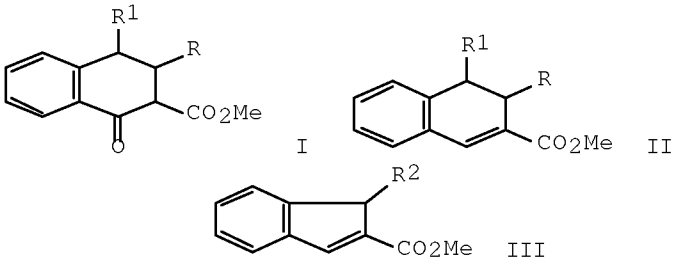


RN 154012-99-4 ZCAPLUS

CN 1H-Indene-2-carboxylic acid, 2,3-dihydro-5-methoxy-1-oxo-3-phenyl-, ethyl ester (CA INDEX NAME)

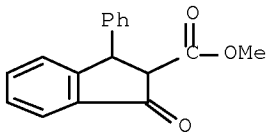


L108 ANSWER 18 OF 21 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1982:562525 ZCAPLUS Full-text
DOCUMENT NUMBER: 97:162525
ORIGINAL REFERENCE NO.: 97:27097a,27100a
TITLE: Synthesis of methoxycarbonylated indenes, 1,2-dihydronaphthalenes, and benzocycloheptene. Preparation of the starting 1-indanones, 1-tetralones, and benzosuberone
AUTHOR(S): Vebrel, Joel; Carrie, Robert
CORPORATE SOURCE: Fac. Sci. Tech., Univ. Franche-Comte, Besancon, F 25030, Fr.
SOURCE: Bulletin de la Societe Chimique de France (1982), (3-4, Pt. 2), 116-24
CODEN: BSCFAS; ISSN: 0037-8968
DOCUMENT TYPE: Journal
LANGUAGE: French
OTHER SOURCE(S): CASREACT 97:162525
GI



AB I (R = Me, CHMe2, Ph, H; R1 = H, Me, CHMe2, Ph) were reduced, and the products were dehydrated to the resp. II; similarly prepared were indenecarboxylate esters III (R2 = H, Me, CHMe2, Ph). 4-Phenylbutyric acids were cyclized to the resp. 1-tetralones, and the latter reacted with Me2CO3 to yield I.
CC 25-24 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
IT 7442-52-6P 66130-38-9P 83303-47-3P 83303-48-4P 83303-49-5P 83303-50-8P 83303-51-9P 83303-52-0P 83303-53-1P 83303-54-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydride reduction of, and dehydration of product from)
IT 83303-48-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydride reduction of, and dehydration of product from)
RN 83303-48-4 ZCAPLUS

CN 1H-Indene-2-carboxylic acid, 2,3-dihydro-1-oxo-3-phenyl-, methyl ester (CA INDEX NAME)



L108 ANSWER 19 OF 21 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1962:12880 ZCAPLUS Full-text
DOCUMENT NUMBER: 56:12880
ORIGINAL REFERENCE NO.: 56:2389h-i,2390c-h
TITLE: Behavior of α-substituted chalcones on attempted Friedel-Crafts arylation
AUTHOR(S): Koelsch, C. F.
CORPORATE SOURCE: Univ. of Minnesota, Minneapolis
SOURCE: Journal of Organic Chemistry (1961), 26, 2590-2
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB cf. CA 55, 19873b. PhCH:CBzCH2CO2H (10 g.) boiled 15 min. with 12 g. AlCl3 in 50 ml. C6H6, the deep orange-red solution decomposed with iced HCl, extracted with dilute Na2CO3, the acidic product (9.4 g.) triturated with Et2O, and crystallized from AcOH gave 3-phenylhydrindone-2-acetic add (I), m. 131-3°. I (0.1 g.) in 1 ml. AcOH gently warmed with 0.06 g. Br with evolution of HBr, the mixture evaporated, the solid boiled with 2% Na2CO3, filtered from 25 mg. waxy material, and acidified yielded 50 mg. 3-phenylindone-2-acetic acid, m. 165-7°. I (1.2 g.) and 6 ml. H2SO4 heated 4 min. on a steam bath, poured onto ice, and the product (0.6 g.) recrystd. from alc. gave 0.4 g. needles of 3,4-benzo-1,2,4a,9a- tetrahydro-2,9fluorenedione (H), m. 165-7°. II (0.8 g.) in 5 ml. AcOH treated with 0.4 g. Br and the dark purple crystalline precipitate recrystd. from 75 ml. AcOH gave 0.55 g. 3,4-benzo-2-hydroxy9-fluorenone (III). III (0.2 g.) boiled in 5 ml. 2% aqueous NaOH, the cooled mixture treated with MeOH, the solution treated alternately with Me2SO4 and NaOH until the latter no longer developed a blue color, filtered, and the precipitate crystallized from EtOAc-ligroine gave 0.2 g. 3,4-benzo-2-meth oxy-9-fluorenone, m. 155-6°. Although formation of I appeared to be anomalous, in contrast to addition of the elements of C6H6 to chaleone (IV), similar reactions occurred with α-methylchalcone (V) and α-phenylchalcone (VI). Careful separation of the addition products of C6H6 and IV allowed isolation of 0.3% 3-phenylhydrindone (VII) in addition to 90% of the normal product, Ph2CHCH2Bz (VIII). AlCl3 (70 g.) in 300 ml. C6H6 treated 15 min. with 100 g. IV (exothermic reaction), the mixture boiled 15 min., the orange-red complex hydrolyzed with ice-HCl, the C6H4 replaced with ligroine (b. 60-70°), filtered from 97 g. almost pure VIII, the mother liquor concentrated, diluted with ligroine, filtered from 21 g. VIII, evaporated, the residue (17.4 g.) separated by fractional distillation, and the fractions chromatographed gave 6.4 g. VIII, 2 g. Ph2CH2, and 0.29 g. VII, m. 76-7°. V (5.5 g.), 4 g. AlCl3, and 20 ml. C6H6 boiled 15 min. and the solution decomposed with ice HCl yielded 5.1 g. 2-methyl-3-phenylhydrindone, b15 1958°, converted by treatment with the calculated amount of Br in AcOH and KOH in MeOH to give quant. 2-methyl-3 phenylindone, m. 83-4°. VI (2.8 g.) and 1.5 g. AlCl3 in 15 ml. C6H6 boiled 2 min. and the isolated product (2.8 g.)

separated by fractional crystallization from alc. gave 0.9 g. 2,3-diphenylhydrindone, m. 98-100°, and 1.3 g. stereoisomeric 2,3° diphenylhydrindone, m. 135-53°, both converted by BrAcOH and KOH-MeOH to 2,3-diphenylindone. Crystalline α-bromochalcone (1.5 g.) boiled 10 min. with 1.5 g. AlCl3 in 10 ml. C6H6 and the isolated product crystallized from alc. gave 1.5 g. 2-bromo-3-phenylhydrindone, m. 84-7°, stereoisomeric with the compound, m. 88-90°, obtained by brominating 3-phenylhydrindone, differing in the infrared spectra by the presence of bands at 765, 745, and 703 cm.-1 in the 87° isomer, in place of bands at 760, 742, and 700 cm.-1 in the 90° isomer. Both gave 3-phenylindone semicarbazone, m. 205° (decomposition). C6H6 (10 ml.) containing 1.5 g. α-carbethoxychalcone and 2 g. AlCl3 boiled 15 min., cooled, and the product (1.45 g.) triturated with Et2O gave 2-carbethoxy-3phenylhydrindone, m. 86-8°, blue-violet with alc. FeCl3, identical with the products obtained by catalytic hydrogenation or Zn-AcOH reduction of 2-carbethoxy-3-phenylindone or by condensation of 3-phenylhydrindone with Et2CO3. It was concluded that a steric effect was responsible for the formation of hydrindones rather than phenylation products.

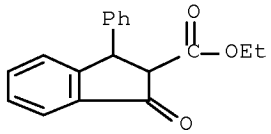
CC 30 (Condensed Aromatic Compounds)

IT 606-86-0P, Propiophenone, 3,3-diphenyl- 7474-64-8P, 1-Indanone, 2,3-diphenyl- 16618-72-7P, 1-Indanone, 3-phenyl- 37758-27-3P, 1-Indanone, 2-bromo-3-phenyl- 52957-74-1P, 1-Indanone, 2-methyl-3-phenyl- 78250-17-6P, 7H-Benzo[c]fluoren-7-one, 5-methoxy- 78250-21-2P, 7H-Benzo[c]fluoren-7-one, 5-hydroxy- 92581-85-6P, Cyclopentanecarboxylic acid, 3-benzyl-2-oxo-, ethyl ester 93321-71-2P, 2-Indanacetic acid, 1-oxo-3-phenyl- 93326-53-5P, Indene-3-carbonitrile, 2-(salicylideneamino)-(?) 93652-16-5P, Cyclopentanecarboxylic acid, 3-cinnamylidene-2-oxo-, ethyl ester 93657-73-9P, o-Toluic acid, α-(3-cyano-2-oxo-1-indanylidene)- 93875-76-4P, 2-Indancarboxylic acid, 1-oxo-3-phenyl-, ethyl ester 94578-53-7P, 1-Indancarbonitrile, 3-cinnamylidene-1-methyl-2-oxo- 95127-15-4P, Cyclopentanecarboxylic acid, 3-benzylidene-2-oxo-, ethyl ester 95276-35-0P, 1-Indancarbonitrile, 2-oxo-3-(3-phenylpropyl)- 95433-62-8P, Cyclopentanecarboxylic acid, 3-cinnamylidene-2-oxo-, ethyl ester, (2,4-dinitrophenyl)hydrazone 98221-17-1P, 7H-Benzo[c]fluorene-5,7-(6H)-dione, 6a,11b-dihydro- 98579-64-7P, o-Tolualdehyde, α-(3-cyano-2-oxo-1-indanylidene)-, semicarbazone 100273-98-1P, Cyclopentanecarboxylic acid, 3-benzylidene-2-oxo-, ethyl ester, (2,4-dinitrophenyl)hydrazone 856346-11-7P, 1-Indancarboxylic acid, 3-(3-phenylpropyl)-, ethyl ester
RL: PREP (Preparation)
(preparation of)

IT 93875-76-4P, 2-Indancarboxylic acid, 1-oxo-3-phenyl-, ethyl ester
RL: PREP (Preparation)
(preparation of)

RN 93875-76-4 ZCAPLUS

CN 1H-Indene-2-carboxylic acid, 2,3-dihydro-1-oxo-3-phenyl-, ethyl ester (CA INDEX NAME)

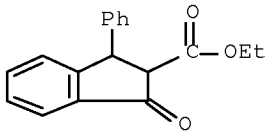


L108 ANSWER 20 OF 21 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1961:105737 ZCAPLUS Full-text
DOCUMENT NUMBER: 55:105737
ORIGINAL REFERENCE NO.: 55:19873b-h
TITLE: An indone to naphthol ring expansion
AUTHOR(S): Koelsch, C. F.
CORPORATE SOURCE: Univ. of Minnesota, Minneapolis
SOURCE: Journal of Organic Chemistry (1961), 26, 1003-5
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB 2-Carbethoxy-3-phenylindone (I) added phenacyl chloride (II) in a Michael reaction and the resulting anion at once eliminated chloride to form Et 1-benzoyl-2-oxo-6b-phenyl-1a,6b-dihydrocycloprop[b]indene-1a-carboxylate (III). III was attacked further by bases, which caused it to rearrange into Et 3-benzoyl-1-hydroxy-4-phenyl-2-naphthoate (IV). I (2.5 g.), 1.5 g. II, and 12 ml. Me3COH warmed, cooled to 25° and the fine suspension treated 15 min. with 0.75 ml. 85% KOH in 1.5 ml. H2O gave 2.6 g. III, flat needles, m. 115-16° (dilute alc.). III (2.6 g.) heated 15 min. with 0.17 g. Na in 5 ml. alc. gave 2.4 g. IV, prisms, m. 120-1° blue with alc. FeCl3. IV refluxed 1 hr. with excess 5% NaOH gave quant. 3-benzoyl-1-hydroxy-4-phenyl-2-naphthoic acid (V), sintered at 195°, m. 215-17° with effervescence. V (0.4 g.) heated 5 min. at 220° gave 3-benzoyl-4-phenyl-1-naphthol (VI), prisms, m. 226° (PhMe); yellow Na salt. Methylation of VI with Me2SO4 in 5% NaOH gave 3-benzoyl-1-methoxy-4-phenylnaphthalene (VIa), plates, m. 148-9° (alc.). Diphenylitaconic acid (15 g.) in 450 ml. 10% NaOH treated under reflux 0.5 hr. with 30 g. Raney Ni, the mixture added to a concentrated solution of 20 g. BaCl2, the salt collected, and refluxed 15 min. with 150 ml. H2O containing 25 ml. HCl gave 14.9 g. benzhydrylsuccinic acid (VII), m. 180-3°. The Al complex, which resulted when the reduction mixture from 10 g. diphenylitaconic acid was poured into hot HCl and refluxed 1 hr. with 50 ml. MeOH containing 5 ml. H2SO4, gave 5.8 g. Me H benzhydrylsuccinate (VIII), m. 150-2° (EtOAcligroine). Me benzhydrylsuccinate (IX) remained in the Et2O and separated to give 3 g. prisms, m. 84-5° (ligroine). Saponification of VIII or IX gave VII. Cyclization of 8.4 g. VII gave 7.3 g. crude 1-phenyl-4-oxo-1,2,3,4- tetrahydro-2-naphthoic acid; Me ester (X) (4.5 g.) m. 115-17° (MeOH). X (4.5 g.) in 10 ml. C6H6 treated with 2.6 g. Br, the residue taken up in 30 ml. collidine, and refluxed 4 min. gave 3.8 g. Me 4-hydroxy-1-phenyl-2-naphthoate (XI), plates, m. 173-4° (MeOH). Methylation of XI with excess Me2SO4 in aqueous alkali gave 86% Me 4-methoxy-1-phenyl-2-naphthoate (XII), needles, m. 118-19° (80% AcOH). XII (1.5 g.) and 0.7 g. NaOH in 6 ml. glycol refluxed 1 min. gave 1.4 g. 4-methoxy-1-phenyl-2-naphthoic acid (XIII), prisms, m. 217-19° (AcOH). XIII (1.4 g.) in 5 ml. C6H6 refluxed 5 min. with 1.2 ml. SOCl2 and the acid chloride shaken 10 min. with 10 ml. NH4OH and C6H6 gave 1.35 g. 4-methoxy-1-phenyl-2-naphthamide (XIV), m. 210-12° soluble in refluxing SOCl2, but recovered unchanged. XIV (1.1 g.) refluxed 10 min. with 5 ml. POCl3 gave 1 g. 4-methoxy-1-phenyl-2-naphthonitrile (XV), m. 162° (AcOH). XV (0.9 g.) in 5 ml. C6H6 refluxed 0.5 hr. with PhMgBr-Et2O gave 1 g. 4-methoxy-1-phenyl-2-naphthyl Ph ketimine-HCl (XVI), prisms, m. 235-40° (MeOH-Et2O). XVI was quite resistant to hydrolysis, but when 0.6 g. XVI was refluxed 15 min. with 5 ml. 50% AcOH containing a trace of HCl it gave 0.5 g. VIa.

CC 10F (Organic Chemistry: Condensed Carbocyclic Compounds)
IT 93875-76-4, 2-Indancarboxylic acid, 1-oxo-3-phenyl-, ethyl ester (reaction with 2-chloroacetophenone)
IT 93875-76-4, 2-Indancarboxylic acid, 1-oxo-3-phenyl-, ethyl ester (reaction with 2-chloroacetophenone)
RN 93875-76-4 ZCAPLUS
CN 1H-Indene-2-carboxylic acid, 2,3-dihydro-1-oxo-3-phenyl-, ethyl ester (CA

INDEX NAME)



L108 ANSWER 21 OF 21 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1951:16487 ZCAPLUS Full-text
DOCUMENT NUMBER: 45:16487
ORIGINAL REFERENCE NO.: 45:2928i,2929a-g
TITLE: Rearrangement of diethyl 3-phenylphthalidyl-3-malonate to derivatives of 3-phenylindone-2-carboxylic acid
AUTHOR(S): Yost, Wm. L.; Burger, Alfred
CORPORATE SOURCE: Univ. of Virginia, Charlottesville
SOURCE: Journal of Organic Chemistry (1950), 15, 1113-18
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 45:16487
GI For diagram(s), see printed CA Issue.
AB Because the lactone ring in phthalein indicators is extremely sensitive to dilute alkali, whereas 3,3-diphenyl- and certain 3,3-dialkylphthalides are stable to acid and bases, a number of 3-alkyl-3-arylphthalides are prepared and the effect of various functional groups in the alkyl group on the stability of the furanone ring is studied. A stream of dried air is passed 20 hrs. over the surface of a mixture of 45.2 g. o-BzC6H4CO2H (I) and 95.2 g. SOCl2 at 50°, then dry air is passed 5 hrs. through the mixture, and the cooled sirupy residue dissolved in 100 cc. ether and added rapidly with stirring to Mg[CH(CO2Et)2]2 from 35.2 g. ester, giving a thick, sirupy, greenish precipitate The mixture is stirred 1 hr., kept overnight, cooled, and decomposed with 130 cc. 37% H2SO4, the ether solution washed with H2O, extracted with 10% Na2CO3 and H2O, the residue dried by distilling it with C6H6 to near dryness, and absolute ether added, giving 24% di-Et 3-phenyl-3-phthalidemalonate (II), crystals from absolute ether, m. 77-9°. Acidification of the washed (ether) Na2CO3 exts. gives a small amount of Et 3-phenylindone-2-carboxylate (III), highly refractive deep yellow crystals, m. 86-7.5°. Distillation of the residue of the ether mother liquors of II in vacuo gives 23.4% III. Warming 10 g. II in 100 cc. 10% Na2CO3 20 min. at 50° and neutralizing the clear solution with 6 N HCl give 88.8% III. Heating 3.68 g. II 1 hr. in 10 cc. AcOH containing 1 cc. H2O and 5 drops concentrated H2SO4 while distilling off the AcOEt formed, diluting the mixture with 20 cc. H2O, extracting it with C6H6, extracting the H2O-washed C6H6 solution with 10% Na2CO3, and acidifying the alkaline solution with 6 N HCl give 100% 3-phenylindone-2-carboxylic acid (IV), brilliant red felted needles, m. 153.5-6°. Hydrogenation of 1.8 g. III in 25 cc. absolute EtOH with Raney Ni at 34° gives crude Et 1-oxo-3-phenyl-2- indancarboxylate, m. 86-7.5°, which, hydrolyzed 1 hr. at 90° with 10 cc. AcOH containing a trace of 50% H2SO4, gives 3-phenyl-1-indanone (V) (semicarbazone, m. 217.5-19.5°). Hydrogenation of 1.28 g. IV in 25 cc. absolute EtOH in the presence of PdCl4 at 34° gives V. Gently refluxing 2.5 g. II 1 hr. in 10 cc. EtOH and 10 cc. 40% KOH, distilling off 30 cc. alc. with simultaneous addition of 30 cc. H2O, extracting the mixture with C6H6, acidifying the alkaline solution with concentrated HCl,

extracting it with C6H6, evaporating the dried extract, and treating the residue with CHCl3 give 3-phenyl-3-phthalideacetic acid, o-C6H4.CO.O.CPhCH2CO2H, m. 175-7°, which is also obtained by refluxing 1 g. 3-allyl-3-phenylphthalide (VI) with 1.7 g. KMnO4 in 20 cc. H2O 35 min. and acidifying the filtered solution with concentrated HCl. Addition of 33.9 g. I in 280 cc. ether over a period of 1.25 hrs. to CH2:CHCH2MgBr from 38.5 g. bromide in 950 cc. ether while simultaneously distilling off ether at the same rate, adding 930 cc. C6H6, distilling off the ether until the temperature of the mixture reaches 80°, refluxing the latter 11 hrs., hydrolyzing it with 100 cc. ice H2O, decanting the liquid from the excess Mg, treating the residue with 300 cc. 9% HCl, and distilling the residue of the washed (H2O, NaHCO3, H2O) and dried C6H6 layer give 57.1% VI, b0.4 168-9.5°, n25D 1.5808, b0.2 153-4°, n25D 1.5848.

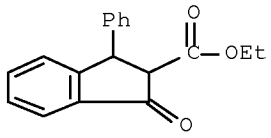
CC 10 (Organic Chemistry)

IT 436-74-8P, 2-Dibenzofurancarboxylic acid, 3-hydroxy-7-methoxy-1-pentyl-9-propyl- 35065-24-8P, 3,7-Dibenzofurandiol 66528-17-4P, 2-Indenecarboxylic acid, 1-oxo-3-phenyl- 93875-76-4P, 2-Indancarboxylic acid, 1-oxo-3-phenyl-, ethyl ester 94224-67-6P, 2-Indenecarboxylic acid, 1-oxo-3-phenyl-, ethyl ester 101278-36-8P, 1-Phthalanacetic acid, 3-oxo-1-phenyl- 860358-14-1P, 1-Indanone, 3-phenyl-, semicarbazone 875228-62-9P, Phthalide, 3-allyl-3-phenyl-
RL: PREP (Preparation)
(preparation of)

IT 93875-76-4P, 2-Indancarboxylic acid, 1-oxo-3-phenyl-, ethyl ester
RL: PREP (Preparation)
(preparation of)

RN 93875-76-4 ZCAPLUS

CN 1H-Indene-2-carboxylic acid, 2,3-dihydro-1-oxo-3-phenyl-, ethyl ester (CA INDEX NAME)



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=>  d his full

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                D SCA
                SEL RN

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L5              STRUCTURE UPLOADED
L6            7 SEA SSS SAM L5
                D SCA
                D STAT QUE L6
L7          427 SEA SSS FUL L5
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L8           45 SEA ABB=ON  PLU=ON  L4 AND L7

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L10             ANALYZE PLU=ON  L9 1- RN HIT :     412 TERMS
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     FILE 'REGISTRY' ENTERED AT 10:04:14 ON 23 JUN 2008
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L12           7 SEA ABB=ON  PLU=ON  L8
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L19          417 SEA ABB=ON  PLU=ON  L9 NOT L18

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L20           99 SEA ABB=ON  PLU=ON  L19

     FILE 'REGISTRY' ENTERED AT 10:34:21 ON 23 JUN 2008
L21              STRUCTURE UPLOADED
L22           14 SEA SUB=L7 SSS SAM L21
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L23              STRUCTURE UPLOADED
L24              STRUCTURE UPLOADED
L25              STRUCTURE UPLOADED
L26           11 SEA SUB=L7 SSS SAM L25
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L30            8 SEA ABB=ON  PLU=ON  L8 NOT L29
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     FILE 'ZCAPLUS' ENTERED AT 10:50:58 ON 23 JUN 2008
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L32            6 SEA ABB=ON  PLU=ON  L29
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     FILE 'REGISTRY' ENTERED AT 10:52:13 ON 23 JUN 2008
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L35              STRUCTURE UPLOADED
L36           14 SEA SUB=L7 SSS SAM L35
                 D SCA
L37              STRUCTURE UPLOADED
L38           13 SEA SUB=L7 SSS SAM L37
L39            1 SEA ABB=ON  PLU=ON  L36 NOT L38
                 D SCA
L40          196 SEA SUB=L7 SSS FUL L37
                 SAVE TEMP BAE913STR37L/A L40
L41            6 SEA ABB=ON  PLU=ON  L27 NOT L40
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     FILE 'ZCAPLUS' ENTERED AT 11:04:22 ON 23 JUN 2008
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                D SCA
L45          55 SEA SUB=L7 SSS FUL L43
L46          40 SEA ABB=ON  PLU=ON  L45 NOT (L40 OR L27)

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L48          34 SEA ABB=ON  PLU=ON  L46

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L49         185 SEA ABB=ON  PLU=ON  L7 NOT (L27 OR L40 OR L45)
                D SCA

     FILE 'ZCAPLUS' ENTERED AT 11:26:34 ON 23 JUN 2008
L50          70 SEA ABB=ON  PLU=ON  L28 OR L42 OR L47

     FILE 'REGISTRY' ENTERED AT 11:27:31 ON 23 JUN 2008
L51          36 SEA ABB=ON  PLU=ON  L7 AND NC2OC2/ESS
L52           9 SEA ABB=ON  PLU=ON  L51 AND >1 C6/ES
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L53           6 SEA ABB=ON  PLU=ON  L52 AND L29
                D SCA

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L57      289180 SEA ABB=ON  PLU=ON  ?ARTER?/BI
L58      504356 SEA ABB=ON  PLU=ON  ?LIPID?/BI
L59      225556 SEA ABB=ON  PLU=ON  ?INSULIN?/BI
L60      124786 SEA ABB=ON  PLU=ON  ?HYPERTENS?/BI
L61       32726 SEA ABB=ON  PLU=ON  ?HYPOTENS?/BI
L62       89940 SEA ABB=ON  PLU=ON  ?OSTEO?/BI
L63      594903 SEA ABB=ON  PLU=ON  LIVER/BI
L64       25633 SEA ABB=ON  PLU=ON  ?CIRRHOS?/BI
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L73      308147 SEA ABB=ON  PLU=ON  ?CARCINO?/BI
L74       44793 SEA ABB=ON  PLU=ON  ?LYMPHOM?/BI
L75       39743 SEA ABB=ON  PLU=ON  ?MELANOM?/BI
L76       51481 SEA ABB=ON  PLU=ON  ?ANGIOGEN?/BI
L77           5 SEA ABB=ON  PLU=ON  L32 AND (L54 OR L55 OR L56 OR L57 OR L58
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                L76)
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                E E2+ALL/CT
L79       23760 SEA ABB=ON  PLU=ON  PEROXISOM?/BI
L80           5 SEA ABB=ON  PLU=ON  L32 AND (L78 OR L79)
L81          12 SEA ABB=ON  PLU=ON  (L28 OR L42) AND (L54 OR L55 OR L56 OR L57
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                OR L67 OR L68 OR L69 OR L70 OR L71 OR L72 OR L73 OR L74 OR L75
                OR L76 OR L78 OR L79)
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                OR L78 OR L79)
L83           182 SEA ABB=ON  PLU=ON  CHEON H?/AU
L84          3187 SEA ABB=ON  PLU=ON  YOO S?/AU
L85         59373 SEA ABB=ON  PLU=ON  KIM S?/AU
L86         21228 SEA ABB=ON  PLU=ON  YANG S?/AU
L87         29002 SEA ABB=ON  PLU=ON  KIM K?/AU
L88          1765 SEA ABB=ON  PLU=ON  RHEE S?/AU
L89          4785 SEA ABB=ON  PLU=ON  AHN J?/AU
L90         12179 SEA ABB=ON  PLU=ON  KANG S?/AU
L91          2087 SEA ABB=ON  PLU=ON  JUNG W?/AU
L92         28054 SEA ABB=ON  PLU=ON  PARK S?/AU
L93          6020 SEA ABB=ON  PLU=ON  KIM N?/AU
L94           102 SEA ABB=ON  PLU=ON  MO K?/AU
L95         67579 SEA ABB=ON  PLU=ON  LEE J?/AU
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L99             6 SEA ABB=ON  PLU=ON  (L83 OR L84 OR L85 OR L86 OR L87 OR L88 OR
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     FILE 'ZCAPLUS' ENTERED AT 11:43:13 ON 23 JUN 2008
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                OR L68 OR L69 OR L70 OR L71 OR L72 OR L73 OR L74 OR L75 OR L76
                OR L78 OR L79)
L101            6 SEA ABB=ON  PLU=ON  L99 OR L100
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     FILE 'ZCAPLUS' ENTERED AT 11:44:58 ON 23 JUN 2008
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                D STAT QUE L77
                D STAT QUE L80
L102            3 SEA ABB=ON  PLU=ON  (L32 OR L77 OR L80 ) NOT L101
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     FILE 'ZCAPLUS' ENTERED AT 11:46:47 ON 23 JUN 2008
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                D STAT QUE L42
                D STAT QUE L81
L103           40 SEA ABB=ON  PLU=ON  (L28 OR L42 OR L81) NOT (L102 OR L101)
L104           14 SEA ABB=ON  PLU=ON  L103 AND ((L47 OR L82))
L105           40 SEA ABB=ON  PLU=ON  L103 OR L014/OBI
L106           40 SEA ABB=ON  PLU=ON  L103 OR L104
                D IBIB ABS HITIND HITSTR L106 1-40
L107            3 SEA ABB=ON  PLU=ON  L102 AND (L28 OR L42 OR L81)
                D IBIB ABS HITIND HITSTR L107 1-3
```

```
     FILE 'REGISTRY' ENTERED AT 11:51:24 ON 23 JUN 2008

     FILE 'ZCAPLUS' ENTERED AT 11:51:27 ON 23 JUN 2008
                D STAT QUE L47
                D STAT QUE L82
L108          21 SEA ABB=ON  PLU=ON  (L47 OR L82) NOT (L101 OR L102 OR L28 OR
                   L42 OR L81)
                D IBIB ABS HITIND HITSTR L108 1-21


     FILE HOME

     FILE REGISTRY
     Property values tagged with IC are from the ZIC/VINITI data file
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